January 2013

The Combined Effects of Light and Temperature on Coral Bleaching: A Case Study of the Florida Reef Tract Using Satellite Data

Brian Burnel Barnes

University of South Florida, bbarnes4@mail.usf.edu

Follow this and additional works at: http://scholarcommons.usf.edu/etd

Part of the Oceanography Commons, and the Other Oceanography and Atmospheric Sciences and Meteorology Commons

Scholar Commons Citation


http://scholarcommons.usf.edu/etd/4863

This Dissertation is brought to you for free and open access by the Graduate School at Scholar Commons. It has been accepted for inclusion in Graduate Theses and Dissertations by an authorized administrator of Scholar Commons. For more information, please contact scholarcommons@usf.edu.
The Combined Effects of Light and Temperature on Coral Bleaching:
A Case Study of the Florida Reef Tract Using Satellite Data

by

Brian Burnel Barnes

A dissertation submitted in partial fulfillment
of the requirements for the degree of
Doctor of Philosophy
College of Marine Science
University of South Florida

Major Professor: Chuanmin Hu, Ph.D.
Pamela Hallock Muller, Ph.D.
Frank Muller-Karger, Ph.D.
David Palandro, Ph.D.
Richard Zepp, Ph.D.

Date of Approval:
November 25, 2013

Keywords: Coral Reefs, Water Clarity, Moderate Resolution Imaging Spectroradiometer, Cloud Detection, Landsat

Copyright © 2013, Brian Burnel Barnes
DEDICATION

This dissertation is dedicated to my wife Samantha and son Isaac. Thank you both for your assistance and unyielding love. Thanks also to my parents Raymond and Annette, as well as to my siblings Michelle, Casey, Diane, Heather, Eric, and Michael for their encouragement and support.
ACKNOWLEDGMENTS

This dissertation would not have been possible without the guidance of Dr. Chuanmin Hu. Thank you for mentoring and supporting me throughout this work. I am thoroughly grateful for your enthusiasm, patience, and commitment to quality science. Thank you also to my committee members, Dr. Pam Hallock Muller, Dr. Frank Muller-Karger, Dr. David Palandro, and Dr. Richard Zepp for their support throughout this process.

Enumerable individuals and groups were instrumental (in scientific capacities or otherwise) towards completion of this dissertation. In particular, I would like to thank my coauthors, as well as friends and colleagues within the Optical Oceanography Lab (especially Jen Cannizzaro, Dave English, and Brock Murch) and the Institute for Marine Remote Sensing (especially Inia Soto, Brendan O’Connor and Sennai Habtes).

This research was made possible, in part, by two grants from the National Aeronautics and Space Administration (NASA) to the University of South Florida, and a grant from NASA to the Environmental Protection Agency and Florida Fish and Wildlife Research Institute. Endowed fellowships from the College of Marine Science, University of South Florida (Anne & Werner Von Rosenstiel Fellowship, Jack & Katharine Ann Lake Fellowship, and William & Elsie Knight Fellowship) provided immeasurable support for this research.
# TABLE OF CONTENTS

LIST OF TABLES ................................................................................................................................. iii

LIST OF FIGURES ............................................................................................................................... iv

ABSTRACT ........................................................................................................................................ v

CHAPTER 1: INTRODUCTION ................................................................................................................. 1
   1. Coral bleaching and environmental stress ............................................................................ 1
      1.1. Temperature ........................................................................................................ 2
      1.2. Light .............................................................................................................. 2
      1.3. Other Factors ............................................................................................... 4
   2. Satellite assessment of coral environments ..................................................................... 5
      2.1. Sea surface temperature ............................................................................. 6
      2.2. Light attenuation ....................................................................................... 8
   3. Study area ....................................................................................................................... 10
   4. Objectives ..................................................................................................................... 12
   5. Approach and dissertation structure ........................................................................... 12
   6. Literature cited ............................................................................................................. 14

CHAPTER 2: IMPROVED CLOUD DETECTION FOR AVHRR AND MODIS SST DATA .................. 23
   1. Research overview .................................................................................................... 23

CHAPTER 3: DEVELOPMENT AND VALIDATION OF SATELLITE-BASED WATER CLARITY PRODUCTS IN THE FLORIDA KEYS ........................................................................................................ 25
   1. Research overview .................................................................................................... 25

CHAPTER 4: PREDICTION OF CORAL BLEACHING USING REMOTELY SENSED SEA SURFACE TEMPERATURE AND LIGHT PENETRATION: A CASE STUDY OF THE FLORIDA KEYS REEF TRACT ........ 27
   Abstract ......................................................................................................................... 27
   1. Introduction ............................................................................................................. 28
   2. Methods .................................................................................................................. 31
      2.1. Data collection and processing ..................................................................... 31
      2.2. In situ data ..................................................................................................... 38
      2.3. Combined environmental and BI data ....................................................... 40
      2.4. Statistical analyses ...................................................................................... 40
   3. Results ..................................................................................................................... 42
   4. Discussion ................................................................................................................. 44
      4.1. Causes of coral bleaching ............................................................................ 44
      4.2. Improvement over SST and DHW for modeling bleaching ....................... 48
      4.3. Model limitations ......................................................................................... 50
4.4. Satellite bleaching product ................................................................. 51
4.5. Future improvements ........................................................................ 53
5. Conclusions ......................................................................................... 55
6. Literature cited.................................................................................... 55

CHAPTER 5: HISTORICAL AND FUTURE ASSESSMENT OF ENVIRONMENTAL PARAMETERS AND
CORAL STRESS USING MULTIPLE SATELLITE INSTRUMENTS ................................................................. 63
1. Introduction ............................................................................................ 63
2. Historical perspective: the use of Landsat and SeaWiFS ....................... 64
3. Look into the future: Continuity of MODIS measurements ....................... 67
4. Literature cited .................................................................................... 68

CHAPTER 6: RESEARCH IMPACTS AND CONCLUSIONS ................................................................. 70
1. Summary of findings ............................................................................. 70
2. Research implications ........................................................................... 72
3. Future work ........................................................................................... 75
3.1. Research directions .......................................................................... 75
3.2. Product delivery ................................................................................ 76
4. Conclusions ........................................................................................... 77
5. Literature cited .................................................................................... 78

APPENDIX A: AN IMPROVED HIGH-RESOLUTION SST CLIMATOLOGY TO ASSESS COLD WATER
EVENTS OFF FLORIDA ............................................................................................................................... 82

APPENDIX B: A HYBRID CLOUD DETECTION ALGORITHM TO IMPROVE MODIS SEA SURFACE
TEMPERATURE DATA QUALITY AND COVERAGE OVER THE EASTERN GULF OF MEXICO .................. 88

APPENDIX C: MODIS-DERIVED SPATIOTEMPORAL WATER CLARITY PATTERNS IN OPTICALLY
SHALLOW FLORIDA KEYS WATERS: A NEW APPROACH TO REMOVE BOTTOM
CONTAMINATION ........................................................................................................................................ 102

APPENDIX D: ESTIMATION OF THE DIFFUSE ATTENUATION COEFFICIENT OF ULTRAVIOLET LIGHT
IN OPTICALLY SHALLOW FLORIDA KEYS WATERS FROM MODIS MEASUREMENTS ......................... 118

APPENDIX E: USE OF LANDSAT DATA TO TRACK HISTORICAL WATER QUALITY CHANGES IN
FLORIDA KEYS MARINE ENVIRONMENTS ......................................................................................... 133

APPENDIX F: AUTHOR CONTRIBUTIONS AND COPYRIGHT CLEARANCES ........................................... 146
LIST OF TABLES

Table 1: Summary of data compiled for this study ................................................................. 32

Table 2: Counts for leave-one-out-cross-validation (LOOCV) of CAP model, using summertime
data........................................................................................................................................... 43
LIST OF FIGURES

Figure 1.1: CRW bleaching alerts (mix of current thermal stress and DHW) for the Florida Keys region. .................................................................................................................................................................................. 7

Figure 1.2: Study region, including boundaries of management areas ................................................................. 11

Figure 4.1: Map of study region, indicating water depth from USGS bathymetry ............................................ 33

Figure 4.2: Time series of environmental and bleaching data at a location in the Middle Keys (24.626 N, 81.108 W) from 2002 to 2013 ................................................................................................................................. 37

Figure 4.3: Histograms showing a) sampling frequency by month, and b) frequency of bleaching index values from FRRP (black ‘+’) and AGRRA (grey ‘x’) surveys ......................................................... 39

Figure 4.4: CAP results .............................................................................................................................................. 44

Figure 4.5: CAP-predicted satellite bleaching (Satellite Bleaching Product, lower panel) for the week of September 24 – 30, 2005 ...................................................................................................................... 47

Figure 5.1: Comparison between concurrent and collocated in situ measured Kd(490) and that calculated from SeaWiFS data using the approach described in Appendix C ........................................ 66

Figure 5.2: Percent difference between SeaWiFS and MODIS data from January 3, 2006 at 5 different wavebands ........................................................................................................................................ 67
ABSTRACT

Coral reefs are greatly impacted by the physical characteristics of the water surrounding them. Incidence and severity of mass coral bleaching and mortality events are increasing worldwide due primarily to increased water temperature, but also in response to other stressors. This decline in reef health demands clearer understanding of the compounding effects of multiple stressors, as well as widespread assessment of coral reef health in near-real time.

Satellites offer a means by which some of the physical stressors on coral reefs can be measured. The synoptic spatial coverage and high repeat sampling frequency of such instruments allow for a quantity of data unattainable by in situ measurements. Unfortunately, errors in cloudmasking algorithms contaminate satellite derived sea surface temperature (SST) measurements, especially during anomalously cold events. Similarly, benthic interference of satellite-derived reflectance signals has resulted in large errors in derivations of water quality or clarity in coral reef environments.

This work provides solutions to these issues for the coral reef environments of the Florida Keys. Specifically, improved SST cloudmasking algorithms were developed for both Advanced Very High Resolution Radiometer (AVHRR; Appendix A) and Moderate Resolution Imaging Spectroradiometer (MODIS) data (Appendix B). Both of these improved algorithms were used to reveal the extent and severity of a January 2010 cold event that resulted in widespread mortality of Florida Keys corals. Applied to SST data from 2010, the improved MODIS cloudmasking algorithm also showed improved quantity of SST retrievals with minimal sacrifice in data quality.

Two separate algorithms to derive water clarity from MODIS measurements of optically shallow waters were developed and validated, one focusing on the diffuse downwelling attenuation coefficient
(K_d, m⁻¹) in visible bands (Appendix C), the other on K_d in the ultraviolet (Appendix D). The former utilized a semi-analytical approach to remove bottom influence, modified from an existing algorithm. The latter relied on empirical relationships between an extensive in situ training dataset and variations in MODIS-derived spectral shape, determined using a stepwise principal components regression. Both of these algorithms showed satisfactory validation statistics, and were used to elucidate spatiotemporal patterns of water clarity in the Florida Keys. Finally, an approach was developed to use Landsat data to detect concurrent MODIS-derived reflectance anomalies with over 90% accuracy (Appendix E). Application of this approach to historical Landsat data allowed for long-term, synoptic assessment of the water environment of the Florida Keys ecosystem. Using this approach, shifts in seagrass density, turbidity increases, black water events, and phytoplankton blooms were detected using Landsat data and corroborated with known environmental events.

Many of these satellite data products were combined with in situ reports of coral bleaching to determine the specific environmental parameters individually and synergistically contributing to coral bleaching. As such, SST and visible light penetration were found to be parsimoniously explaining variance in bleaching intensity, as were the interactions between SST, wind and UV penetration. These relationships were subsequently used to create a predictive model for coral bleaching via canonical analysis of principal coordinates. Leave-one-out-cross-validation indicated that this model predicted ‘severe bleaching’ and ‘no bleaching’ conditions with 64% and 60% classification success, respectively, nearly 3 times greater than that predicted by chance. This model also showed improvement over similar models created using only temperature data, further indicating that satellite assessment of coral bleaching based only on SST data can be improved with other environmental data. Future work should further supplement the environmental parameters considered in this research with databases of other coral stressors, as well as improved quantification of the temperature at the depth of corals, in order to gain a more complete understanding of coral bleaching in response to environmental stress.
Overall, this dissertation presents five new algorithms to the field of satellite oceanography research. Although validated primarily in the Florida Keys region, most of these algorithms should be directly applicable for use in other coastal environments. Identification of the specific environmental factors contributing to coral bleaching enhances understanding of the interplay between multiple causes of reef decline, while the predictive model for coral bleaching may provide researchers and managers with widespread, near real-time assessments of coral reef health.
CHAPTER 1:
INTRODUCTION

1. Coral bleaching and environmental stress

When stress becomes extreme, zooxanthellate corals will sometimes expel their algal symbionts (zooxanthellae), causing ‘bleaching’ of the coral tissues (Jokiel and Coles, 1977; Douglas, 2003). In the absence of these symbionts, some corals can survive for periods of time (depending on the species and location), and even re-acquire zooxanthellae after the passing of the stressor (Lasker et al., 1984; Buddemeier and Fautin, 1993). Severe bleaching of coral tissues, however, is often a precursor to reduced energetic capabilities and / or death of all or part of the colony (Glynn, 1996; Hoegh-Guldberg, 1999). The adaptive bleaching hypothesis (Buddemeier and Fautin, 1993) proposes that such expulsions of zooxanthellae allow corals to subsequently re-aquire a more tolerant clade of *Symbiodinium*, resulting in greater fitness of the holobiont. Nevertheless, the overall frequency and severity of bleaching events appears to be increasing (Wilkinson, 1999).

Oxidative stress due to photoinhibition is generally thought to be the primary physiological driver of coral bleaching (Lesser, 1997, 2006). Briefly, when a stressor reduces the photosynthetic electron transport chain efficiency and conditions exist such that pigments continue to absorb light energy, toxic oxygen free radicals can be produced (Lesser, 2006). If the concentration of these reactive oxygen species overwhelms the natural anti-oxidants, then corals may rid themselves of the zooxanthellae either through exocytosis or apoptosis of host cells (Lesser and Farrell, 2004). Hermatypic corals and their symbiotic zooxanthellae have evolved some mechanisms to mitigate the effects of this
oxidative stress, including mycosporine-like amino acids (MAAs; Shick 2004; Ayoub et al., 2012) and fluorescent proteins (Hoegh-Guldberg and Jones, 1999; Brown et al., 1999; Salih et al., 2000).

1.1. Temperature

The temperature of the water surrounding corals can greatly affect their health, as extreme water temperatures can result in bleaching of coral tissues and often subsequent death (Jokiel and Coles, 1977, 1990; Glynn and D’Croz, 1990; Glynn, 1993; Brown, 1997). Even though corals generally live in tropical ecosystems, they tend to be concentrated in areas that are at or near their upper thermal limits (Jokiel and Coles, 1990). Examples abound of 2-3°C increases in temperature causing extensive bleaching of coral tissues (Hoegh-Guldberg, 1999; Goreau et al., 2000; Jokiel and Brown, 2004; Lesser, 2004). Bleaching and mortality of corals (Shinn, 1966; Hudson et al., 1976; Porter et al., 1982; Davis, 1982; Walker et al., 1982; Lirman et al., 2011) and other cnidarians (Steen and Muscatine, 1987; Coles and Fadlallah, 1991) have also been observed during extremely low temperature events. Unfortunately, corals which have shown resiliency to warm temperature-related bleaching and mortality are those most affected by subsequent cold events (Lirman et al., 2011).

Anomalous temperatures, however, are not the sole cause of coral bleaching. Although temperature is thought to be the primary stressor on corals (Lesser and Farrell, 2004), other parameters (e.g., UV radiation) can independently cause bleaching or death (Lesser et al., 1990). When acting in concert with thermal stress, these other environmental stressors have been observed to effectively decrease the temperature threshold for bleaching (Lesser, 2006; Wooldridge, 2009).

1.2. Light

Ambient light is critical for photosynthesis and therefore healthy growth of zooxanthellate corals. However, corals and reef-dwelling foraminifera bleach more readily when exposed to high
energy, short wavelength [blue and ultraviolet (UV, 200 – 400 nm)] radiation (Siebeck, 1988; Fitt and Warner, 1995; Brown, 1997; Lesser, 1997; 2006; Williams and Hallock, 2004). Further, UVB (280 – 315 nm) and UVA (315 – 400 nm) exposure, can cause damage to corals via DNA alterations (Dunne and Brown, 1996; Shick et al., 1996; Sinha and Häder, 2002) or photoinhibition (Fitt and Warner, 1995; Lesser and Lewis, 1996; Ferrier-Pages et al., 2007), respectively. Goenaga et al. (1989) noted that bleaching localized to only the upper surfaces of corals demonstrates an effect of light radiation on coral bleaching, as shading from incident radiation offers some protection from bleaching to the underlying corals. Gleason and Wellington (1993) found that regardless of temperature, given calm waters and clear seas, Caribbean corals transported from 24m to 12m showed bleaching after only 21 days, while similarly transplanted corals which were shaded from UV light by an acrylic cover showed no signs of bleaching. Similarly, Lesser (1997) found decreased photosynthetic performance leading to bleaching of *Agricia tenuifolia* in response to temperature stress and solar radiation, while no reaction to these stressors was seen when corals were exposed to exogenous antioxidant treatments.

In addition to these *in situ* experiments, many natural experiments have given further evidence as to the effect of light on coral health. For example, Mumby et al. (2001) found that cloud cover may have reduced solar irradiance at Society Island, Tahiti, resulting in decreased coral bleaching relative to surrounding areas. Similarly, increased turbidity was attributed to reduced bleaching and mortality of corals relative to adjacent optically clear waters during a widespread bleaching event (Goreau et al., 2000) due to blocking of incoming UV radiation. Other studies have suggested that increased light availability resulting from low tides and / or calm winds led to coral bleaching (Glynn, 1968; Jaap, 1979; Fisk and Done, 1985; Harriott, 1985; Oliver, 1985; Jones, 1997; Hendee et al., 2001). Corals in areas of increased water flow generally have higher stressor resistance and faster recovery from disturbances (West and Salm, 2003) perhaps due to clearer waters, high light transmittance and reduced specular reflection in calm seas (Hendee, 1998).
In addition, light penetration to the benthos is also influenced by biochemical processes in the water column, such as phytoplankton blooms and colored (chromatophoric) dissolved organic matter (CDOM) dynamics. Excess nutrients and subsequent phytoplankton blooms decrease the transparency of the water column, thereby reducing the photosynthetic capabilities of benthic organisms, including corals (Hallock and Schlager, 1986). For example, widespread coral mortalities were identified during an upwelling event (i.e., no thermo-stress) as a result of iron enrichment from nearby wildfires causing a massive red tide and coral asphyxiation (Abram et al., 2003). Tolerance of corals to incident UV radiation may depend on the concentration of CDOM within the surrounding water column (West and Salm, 2003; Zepp et al., 2008) while large-scale climate changes may increase the overall UV radiation reaching corals (Gleason and Wellington, 1993).

1.3. Other Factors

Despite the fact that light and temperature seem to be the primary causative agents of coral bleaching, several other environmental factors may be influencing the health of coral ecosystems (Hoegh-Guldberg, 1999; McManus and Polsenberg, 2004). Wooldridge (2009) found increased bleaching susceptibility in high nutrient waters. Low salinity waters have also been found to cause coral bleaching and mortality (Goreau, 1964) following a hurricane induced flood. Although small amounts of sedimentation can adversely affect corals (Philipp and Fabricius, 2003), turbidity may provide protection from bleaching (Goreau et al., 2000). Extreme low tide events can cause bleaching through aerial exposure of corals (Vaughan, 1911; Loya, 1976). Finally, some diseases have even been identified as causative agents for bleaching (Kushmaro et al., 1996).
2. Satellite assessment of coral environments

Much of the research on coral tolerance to these physical parameters consists of laboratory manipulations of specific coral species, often utilizing extreme shifts in temperature or irradiance, the rate and duration of which may not be realistic for natural environments (see Hoegh-Guldberg and Smith, 1989). *In situ* experiments are extremely difficult to conduct or interpret due to inadequate replication, lack of suitable control sites, and widely unstable random variables.

As understanding of the factors influencing corals increases, shortcomings in ability to assess and/or monitor these parameters over wide time and space scales become obvious. Where quality investigations of causes of reef decline do exist, the scope of the observation tends to be notably localized in space and time (Hughes and Connell, 1999). This deficiency is typically due to financial constraints, which also plague long term programs to monitor the environmental conditions around coral reefs. For example, moored sensor payloads have been deployed to great effect in some coral regions [e.g., Integrated Coral Observation Network (ICON); Hendee *et al*., 2007], but purchase and maintenance of such instrument suites is often expensive (only 1 of 5 ICON subsurface light recording stations in the entire Caribbean region is currently operational). Similarly, maintenance expenses contributed to the demise of Florida Institute of Oceanography’s (FIO) Sustained Ecological Research Related to the Management of the Florida Keys Seascapes (SEAKEYS; 1989 – 2010) monitoring stations and led to dismantling of established instrument suites. Measuring environmental conditions in coral reef regions from regular ship-borne excursions can increase the spatial resolution of monitoring efforts, but often costs of ship time lead to very low temporal resolution.

Through advances in satellite products and algorithms, many of the causative factors for declines in coral reef health listed above can be measured from currently operational satellite instruments. The synoptic spatial scale and high repeat sampling frequency afforded by such satellite sensors dwarfs that which is feasible from *in situ* surveys. Furthermore, applied to the entire time series
of data from a particular instrument, such advances can provide historical assessment of coral stressors
which would be otherwise unattainable. Validated detection of the environmental parameters
surrounding corals from satellites would thus allow for 1) determination of the specific factors (and their
interactions) contributing to coral stress, and 2) synoptic assessment of coral bleaching stress in near
real time.

2.1. Sea surface temperature

As a result of coral responses to elevated temperatures, management and monitoring of coral
environments from satellite data currently focuses on Degree Heating Weeks (DHW). This index is a
measure of water temperature relative to the historical average at a particular location, and depends
both on the length and severity of the disturbance (Gleeson and Strong, 1995). For example, 2 DHWs
could refer to either 2 weeks at 1° C above, or 1 week at 2° C above the maximum monthly mean
(MMM). DHW accumulate over a twelve week running total for each pixel. The global threshold at
which bleaching has been found to occur is 4 DHW, while widespread bleaching and mortality is
expected for regions experiencing 8 DHW (Skirving et al. 2006). Currently this information is used by the
National Oceanic and Atmospheric Administration (NOAA) Coral Reef Watch program (CRW) to chart
DHW values for coral sites, thus providing regular, quick-return information on potentially stressed
environments, available online at http://coralreefwatch.noaa.gov (Strong et al., 2004; Mumby et al.,
2004).

Despite the successes of this algorithm (Skirving et al. 2006), the primary deficiency is that the
currently operational product has a pixel resolution of 0.5 degrees (approx 50 km). This resolution is
achieved by weighted pixel averaging of nighttime Advanced Very High Resolution Radiometer (AVHRR)
global area coverage (GAC) SST data, which have a native resolution of 4km. The purpose of this spatial
binning is to minimize the number of missing pixels due to cloud contamination. Not only does such
coarse resolution ignore small-scale SST heterogeneity, the current DHW product provides no
information for many coastal systems due to mixed land-water pixels. Indeed, virtually no CRW DHW
information is produced for many coastal coral ecosystems, including the Florida Keys (Fig. 1.1). As such,
the current CRW DHW is primarily useful in monitoring potential for mass bleaching events at large
synoptic scales. Efforts are currently ongoing to improve the spatial resolution of the CRW bleaching
products (Vega-Rodriguez et al., 2012; Vega-Rodriguez et al., in prep).

Figure 1.1: CRW bleaching alerts (mix of current thermal stress and DHW) for the Florida Keys region.
The red line represents the approximate boundary of the Florida Reef Tract (FRT). Note that the pixel
size precludes stress quantification for most of the reef. The flagged pixels are virtual monitoring
stations for FRT regions. Note their distance from the corals they are monitoring.

Weeks et al. (2008) found the DHW products insufficient to predict coral bleaching in the
southern Great Barrier Reef. Use of higher resolution SST products and a seasonally adjusted
temperature threshold for bleaching (as opposed to summer MMM) improved the correlation between
the DHW product and coral bleaching instances. Nevertheless, the extent of coral bleaching was not
proportional to the DHW, which the authors propose could be due to seasonal differences in SST thresholds, or may hint at a missed co-variable such as light availability.

The need for higher resolution assessment of coral thermal stress from satellites requires improvement in the cloud detection algorithms for SST data. Cloud detection algorithms for SST products use a variety of methods to determine if a pixel is contaminated by clouds; among them are difference from expected brightness in certain thermal infrared wavelengths, deviation from climatological norms, and combinations thereof (Franz, 2006; Hu et al., 2009; Ackerman et al., 2010). For daytime satellite passes, cloud detection algorithms can also rely on the high reflectance of clouds in all visible bands (e.g., SeaDAS Level 2 Processing Flag CLDICE; Patt et al., 2003). Nevertheless, current cloud detection algorithms are insufficient to fully remove cloud effects from SST datasets while retaining as many valid data as possible. In particular, cloudy pixels are often improperly determined to be valid SST, thereby resulting in negatively biased SST datasets. Alternatively, and especially during anomalously cold events, valid SST data are discarded as clouds. As a result, climatologies overestimate the true average SST for a particular region, which can further perpetuate errors in discrimination between clouds and valid SST during cold events. Improvement of these algorithms is critical for accurate assessment of high-resolution temperature data (and thereby coral stress) and is thus an integral part of this work.

2.2. Light attenuation

Extraterrestrial solar irradiance in the visible and UV is generally constant (in the absence of sun spots), but light reaching Earth’s atmosphere will vary according to the distance between the Sun and Earth. The amount of this radiation that reaches Earth’s surface is primarily a function of solar angle, ozone, atmospheric aerosols and cloud cover. Solar angle is calculable for any point and time on Earth, and does not need to be directly measured. Every 1% decline in atmospheric ozone roughly equates to
a 2% increase in incident UV-B radiation (Shick et al., 1996; Moran et al., 2000; Hallock, 2005). The National Atmospheric and Space Administration’s (NASA’s) satellite ozone measures began in 1978 using the Total Ocean Mapping Spectrometer, and continue today with the Ozone Monitoring Instrument aboard the Aura satellite. Combined with the extraterrestrial solar irradiance, these measurements can be used to estimate the UV light available at the water surface. For the visible wavelengths, photosynthetically available radiation (PAR; integrated 400 to 700 nm) just below the water surface is calculated as one of the standard NASA products from MODIS data (Carder et al., 2003).

Once this light enters the water column, the diffuse attenuation coefficient for downwelling irradiance \( (K_d, \text{ m}^{-1}) \) defines the penetration of light to depth. The amount of UV radiation reaching the benthos is primarily a function of CDOM concentration (Bricaud et al., 1981) and water depth (Clarke and James, 1939), but also is affected by particulate chlorophyll and detritus (Nelson and Guarda, 1995). Their relative contributions to light attenuation, however, are not constant in either space or time (Boss et al., 2001). To complicate this relationship, CDOM also photobleaches under exposure to UV light (Moran and Zepp, 1997; Häder et al., 1998; Shank et al. 2010a), meaning its contribution to attenuation will decrease with constant incident light. As such, without frequent and reliable \( K_d \) estimates, as well as accurate raster bathymetric data, satellite measures of surface radiation tell very little about the light field reaching coral tissues.

Many satellite products have been developed to estimate \( K_d \) (e.g., Austin and Petzold, 1981; Mueller, 2000; Z. Lee et al., 2002; 2005; Morel et al., 2007). However, these products were designed for use on optically deep water targets (where reflection from the bottom is negligible). In optically shallow environments, reflection from the benthos contributes to the reflectance measured from above-water (e.g., satellite) sensors. This contribution is dependent on \( K_d \), benthic albedo, and bottom depth, and thus is spatially, temporally, and spectrally variable. As such, current \( K_d \) algorithms are not directly applicable for coral reef environments in optically shallow waters. Errors in derived water properties for
optically shallow environments, however, can be alleviated through use of longer (red) wavelengths (e.g., Carder et al., 2005), for which less bottom contribution of reflectance is expected. Such an approach can be used to calculate $K_d$ in visible wavelengths for optically shallow waters. However, as current ocean color satellites do not include UV bands, estimation of $K_d$(UV) requires an approach that is resilient to bottom reflectance contribution and that can be extrapolated from visible reflectance data.

3. Study area

The Florida Keys are a 120 mile long string of limestone islands located south of the Florida peninsula. Tourism generates nearly 1.2 billion dollars for the region annually, with approximately 2.5 million visitors annually inundating the region with just over 73,000 permanent residents (US Census Bureau 2011). Among the draws to the region are the marine ecosystems, including the Florida Reef Tract (FRT). The FRT is a string of coral bank and patch reefs located approximately 3 to 10 km east and south of the Florida Keys, covering approximately 1400 km$^2$. Protection of these reefs was one of the factors contributing to the 1990 creation of the Florida Keys National Marine Sanctuary (FKNMS; Causey, 2002). The FKNMS encompasses 9600 km$^2$ of marine waters enveloping the Florida Keys, including most of the FRT (Fig. 1.2).

Traditionally, the Florida Keys have been delineated into regions according to their general circulation patterns (see Klein and Orlando, 1994). Currents generally flow northeastward in the Upper Keys owing to the proximity of the Florida Current. The Lower Keys typically see westward flow due primarily to the easterly winds as well as occasional eddies associated with the Florida Current. The Middle Keys are the transition zone, but they also experience (along with the Lower Keys) inundation with water from Florida Bay and the Southwest Florida Bight through several tidal channels separating the islands (Smith, 1994; T. Lee and Williams, 1999; Porter et al., 1999; T. Lee and Smith, 2002; Smith and Pitts, 2002; T. Lee, 2012).
As has been seen for many Caribbean reefs, FRT coral cover has been in decline for several decades (Hughes, 1994; Palandro et al., 2001; 2008; Andréfouët et al., 2002). Much of this decline has been attributed to extreme temperature events (Jaap, 1985; Warner et al., 1999; Lirman et al., 2011) and water quality changes (Hu et al., 2003; Lapointe et al., 2004). Although corals are typically not found in close proximity to the tidal channels between Keys islands due to unfavorable water conditions (Ginsburg and Shinn, 1964; 1993), the growth rate and coral cover on nearshore FRT reefs has recently been found to significantly exceed those of offshore, more oligotrophic reefs (Lirman and Fong, 2007). One explanation is that corals can benefit from the increased UV attenuation provided by higher CDOM concentrations from Florida Bay and nearshore mangroves (Shank et al., 2010b).
4. Objectives

The overarching goals of this research were to advance satellite remote sensing technology through developing water quality data products for shallow water ecosystems, and to improve our understanding of the connection between physical and bio-chemical water quality parameters and coral bleaching. Towards these goals, the specific research objectives were:

1) Create improved high-resolution satellite SST data products through refining and tuning of cloud detection algorithms for AVHRR and MODIS data.

2) Develop improved UV and visible water clarity algorithms for MODIS and Landsat Thematic Mapper (TM) data.

3) Use these products to further quantify the relationship between coral bleaching and concurrent light and temperature conditions at the benthos.

4) According to results from objective 3, combine light and temperature products described above to develop a comprehensive coral bleaching index from satellite data in near-real time.

5. Approach and dissertation structure

This dissertation is arranged in chapters that detail the research conducted to fulfill these objectives. Chapter 2 focuses on SST cloudmasking (Objective 1) for AVHRR and MODIS data. For both instruments, current cloud detection techniques were assessed and found to be insufficient to reliably differentiate valid SST from clouds, especially during cold water events. As such, new algorithms were developed to improve the SST data coverage and quality, from which the effects of extreme cold events on marine ecosystems (including corals) could be more accurately assessed.
Assessment of $K_d$ (Objective 2) in the optically shallow Florida Keys environment required development of approaches resilient to benthic contribution to satellite-derived reflectance. This work was completed for both visible and UV wavelengths using MODIS data, as detailed in Chapter 3. Briefly, a semi-analytical approach was developed to remove benthic contributions from satellite estimates of $K_d$ in the visible MODIS bands. Alternatively, an empirical approach was developed to derive $K_d$(UV), based on relationships between MODIS-derived spectral shape and concurrent in situ measures.

Chapter 4 details an assessment of bleaching stress (Objective 3) according to remotely sensed environmental parameters. Here, the approach was to use the MODIS $K_d$ and SST algorithms (developed in Chapters 2 and 3), combined with in situ reports of coral bleaching, to quantify the relationship between coral bleaching and concurrent light and temperature conditions. Subsequently, these relationships were used to assess coral bleaching potential from satellite data (Objective 4).

Much of this research relies heavily on data from MODIS on the satellite Aqua, which has already more than doubled its design life. However, coral bleaching has been prevalent in the Keys prior to MODIS coverage, and will continue to be an issue after MODIS eventually fails. Chapter 5 details efforts to derive water quality information from historical TM data (Objective 3). Future research must similarly strive to improve detection of the light and temperature environments surrounding corals from historical, current, and future satellite sensors. In particular, continuity of these measurements must be assured for the recently launched Visible Infrared Imager Radiometer (VIIRS), towards continued improvement in coral reef health assessment from satellite data.

Finally, Chapter 6 summarizes the work detailed in the previous chapters, with particular focus on the implications of the dissertation as a whole. Overall impressions are offered on the successes and failures of this work and lessons learned. Chapter 6 finishes with descriptions of future research directions which would broaden the findings of this work and enhance assessment of coral reefs using satellite data.
6. Literature cited


Vega-Rodriguez, M., Müller-Karger, F.E., Li, J., Eakin, C.M., Guild, L., Hu, C., Lynds, S., Heron, S., Quiles-Perez, GA. (2012). Developing high-resolution thermal stress indices to enhance regional coral bleaching forecasts through NOAA’s Coral Reef Watch decision-support-system. Poster presentation, Ocean Sciences Meeting, Salt Lake City, UT, USA, 2 February 2012.


CHAPTER 2:

IMPROVED CLOUD DETECTION FOR AVHRR AND MODIS SST DATA

1. Research overview

Appendix A – An improved high-resolution SST climatology to assess cold water events off Florida

Cold water events have resulted in mortality of corals, sea turtles, manatees, seagrasses, and many other fauna and flora of the waters surrounding Florida. Cloud detection techniques for satellite data are often insufficient to differentiate between anomalously cold sea surface temperature (SST) and pixels contaminated by clouds. Indeed, nearly 20% of Advance Very High Resolution Radiometer (AVHRR) SST images from the month of January (1995-2010) showed improper cloud masking. Manually delineated overrides of improperly masked regions were used to create an improved SST climatology. This climatology showed the location of negative anomalies throughout Florida waters (up to 14 °C in Florida Bay) during the January 2010 cold event that had previously been masked.

Appendix B – A hybrid cloud detection algorithm to improve MODIS sea surface temperature data quality and coverage over the eastern Gulf of Mexico

Several algorithms have been developed previously by various groups to identify cloud-contaminated pixels from Moderate Resolution Imaging Spectroradiometer (MODIS) SST data. The performance of four algorithms was tested for MODIS SST data from 2010...
covering the eastern Gulf of Mexico using concurrent *in situ* measured SST. None was found to reliably distinguish valid SST from cloud-contaminated data, especially during anomalously cold events. A hybrid algorithm was developed to use these existing algorithms in various combinations according to time and location, based on their observed strengths and weaknesses. While retaining nearly the same high SST accuracy, the hybrid algorithm showed a nearly 20% increase in SST retrievals over the current community standard algorithm.
CHAPTER 3:
DEVELOPMENT AND VALIDATION OF SATELLITE-BASED
WATER CLARITY PRODUCTS IN THE FLORIDA KEYS

1. Research overview

Appendix C – MODIS-derived spatiotemporal water clarity patterns in optically shallow Florida Keys waters: A new approach to remove bottom contamination

This study presents development and validation of a new approach to derive diffuse downwelling attenuation coefficient (\(K_d\), m\(^{-1}\)) data in optically shallow waters for the visible Moderate Resolution Imaging Spectroradiometer (MODIS) bands, using a modification of an existing algorithm. Compared to in situ data, water clarity derived using this modified algorithm showed strong matchup statistics [for \(K_d\)(488) from 0.02 to 0.2 m\(^{-1}\), \(N=22\), \(R^2 = 0.68\), unbiased RMS = 31%] and improvement over current products when compared to the same data (\(N = 13\), \(R^2 = 0.37\), unbiased RMS = 50%). This modified algorithm was subsequently applied all MODIS Aqua data from 2002 – 2011 covering the Florida Keys region. As such, spatiotemporal patterns in water clarity were identified, such as strong onshore-offshore gradients throughout the Florida Keys, consistent with previous reports. The Dry Tortugas region was found to have the clearest water, while the Marquesas region showed the highest \(K_d\) in the Florida Keys. This latter finding contradicts some previously published reports indicating that the Middle Keys have the highest \(K_d\), but agrees with regional water clarity patterns predicted by the local circulation regime.
Appendix D – Estimation of diffuse attenuation of ultraviolet light in optically shallow Florida Keys waters from MODIS measurements

Estimation of $K_d$ in optically shallow waters from MODIS remote sensing reflectance ($R_{RS}$) data requires an approach that is unaffected by benthic reflectance contribution to the satellite derived signal. Also, as MODIS records no ultraviolet (UV) data, derivations of $K_d$(UV) from MODIS must rely on visible MODIS bands. As such, variation in MODIS-derived $R_{RS}$ spectral shapes were tied to concurrent in situ measured $K_d$(UV) in the Florida Keys via a stepwise principal components regression. This approach improves on previously published methods to estimate water parameters using principal components analysis of $R_{RS}$ through the addition of a stepwise forward addition procedure, ensuring parsimonious model selection. Using an extensive collection of in situ $K_d$(UV) data, this approach showed strong model performance [$K_d$(305) ranging from 0.28 to 3.27 $m^{-1}$; $N = 29$; $R^2 = 0.94$] and predictive capabilities, assessed using leave-one-out-cross-validation [for $K_d$(305), $R^2 = 0.92$; bias = $-0.02$ $m^{-1}$; unbiased RMS = 23%].

Applied to the 2002-2012 MODIS dataset, this approach allowed for assessment of the spatiotemporal patterns in $K_d$(UV) in the Florida Keys. While the spatial patterns in $K_d$(UV) generally mimic those of $K_d$ in visible bands [$K_d$(VIS)], the seasonal cycle of $K_d$(UV) shows highest transparency in the winter relative to the summer for much (but not all) of the study area, which is the reverse of the $K_d$(VIS) seasonality. These differences between $K_d$(UV) and $K_d$(VIS) highlight the need for assessment (either in situ or remotely sensed) of $K_d$ in both the UV and visible.
CHAPTER 4:
PREDICTION OF CORAL BLEACHING USING REMOTELY SENSED SEA SURFACE TEMPERATURE AND LIGHT PENETRATION: A CASE STUDY OF THE FLORIDA KEYS REEF TRACT

Abstract

Coral bleaching has been attributed to several physical variables of the coral habitat, in particular extremes in temperature and high ultraviolet radiation. Satellite observing systems and algorithm improvements allow synoptic-scale monitoring of coral environments, which can be used to investigate the individual and synergistic effects of various environmental parameters in causing coral bleaching. Shallow-water algorithms for light penetration, long-term (2002-2013) satellite data, *in situ* bleaching surveys (N = 1712; spanning 2003-2012), and other environmental variables were used to identify the environmental factors contributing to bleaching of Florida Reef Tract corals. As such, a stepwise multiple linear regression indicated that elevated sea surface temperature (SST; partial $R^2_{adj} = 0.13$; $p < 0.001$) and high visible benthic available light (partial $R^2_{adj} = 0.05$; $p < 0.001$) each independently contributed to summertime coral bleaching. The effect of SST was further influenced by significant interactions with both wind speed (partial $R^2_{adj} = 0.03$; $p < 0.001$) and ultraviolet benthic available light (partial $R^2_{adj} = 0.01$; $p = 0.012$). These relationships were then combined via canonical analysis of principal coordinates to create a predictive model of coral reef bleaching for the Florida Keys Reef Tract. This model correctly predicted ‘severe bleaching’ and ‘no bleaching’ conditions with 68% and 59% classification success, respectively. The classification success for these two categories is nearly 3 times greater than that predicted by chance, and also shows improvement over similar models created
using only temperature data. Together, these results lead to a greater understanding of the factors contributing to coral bleaching and allow for weekly prediction of historical and current bleaching stress from satellite data.

1. Introduction

Coral reefs are in decline worldwide due to a multitude of factors (Wilkinson, 1999). Many of the stressors on coral reefs are changes or extremes in physical variables that impact coral habitats (see reviews by Brown, 1997; Hoegh-Guldberg, 1999; Douglas, 2003). Under stress, hermatypic corals may expel symbiotic zooxanthellae, leading to bleaching of the coral tissues (Jokiel and Coles, 1977). Bleaching is not obligatorily fatal, and instead may be a mechanism through which a more tolerant clade of zooxanthellae may be acquired (Buddemeier and Fautin, 1993). Nevertheless, reduced energetic capabilities and a weakened immune system can lead to disease and death of coral tissues during bleaching events (Glynn, 1996; Hoegh-Guldberg, 1999).

Elevated temperatures are considered a dominant cause of coral bleaching worldwide (Jokiel and Coles, 1977, 1990; Glynn and D’Croz, 1990; Glynn, 1993; Brown, 1997; Hoegh-Guldberg, 1999; Goreau et al., 2000; Jokiel and Brown, 2004; Lesser, 2004; and many others). Much evidence suggests that other factors, especially in concert with elevated temperatures, can exacerbate or mitigate coral bleaching in response to thermal stress (Lesser et al., 1990; Lesser, 2006). Of particular relevance are ultraviolet radiation (UV; 280 – 400 nm; Siebeck, 1988; Gleason and Wellington, 1993; Fitt and Warner, 1995; Shick et al., 1996; Lesser, 1997, 2006; Lesser and Farrell, 2004; Williams and Hallock, 2004; Ferrier-Pages et al., 2007) and photosynthetically available radiation (PAR; integrated 400-700 nm; Lesser 1989; Lesser and Shick 1989; Lesser et al., 1990; Osmund 1994; Gleason and Wellington, 1995; Mumby et al., 2001). Generally, these environmental stressors have been observed to decrease the temperature threshold at which coral bleaching occurs (Lesser, 2006; Wooldridge, 2009).
Photoinhibition of coral zooxanthellae has been observed as soon as 24 hours (Fitt and Warner 1995) to 5 days (Ferrier-Pages et al., 2007) after exposure to an increase in UV irradiation. Lesser and Farrell (2004) found that 10 days was sufficient for coral acclimation to a particular irradiance regime, while Ferrier-Pages et al. (2007) found that corals increased production of photoprotective micosporine-like amino acids (MAAs; see Dunlap and Shick, 1998; Shick, 2004) within 14 days of UV exposure. Gleason and Wellington (1993) found that corals transplanted from 24 to 12 m water depth showed bleaching within 7 days (persisting at least 21 days), while transplanted corals covered by a UV filter showed no signs of bleaching. In laboratory experiments, Siebeck (1988) noted an interaction between UV and visible (VIS; 400-700 nm) light, whereby negative responses to UV irradiation were mitigated by concurrent exposure to VIS light. In natural environments, this could indicate that clouds (transparent to UV, yet opaque to VIS) may increase potential bleaching (but see Mumby et al., 2001). Yentsch et al. (2002) found that some reefs are near their minimum thresholds for photosynthetically active radiation (PAR; integrated 400 – 700 nm) reaching coral tissues, below which respiration exceeds photosynthesis. Gleason and Wellington (1995) found non-fatal bleaching of coral larvae in response to increased PAR, whereas no such effect of UV light was detected.

Goenaga et al. (1989) posited that severe coral bleaching is restricted to only the upper surfaces of coral colonies (i.e., the tissues exposed to the strongest irradiation), demonstrating the synergistic effects of light and temperature in causing coral bleaching. More recently, numerous studies have attempted to quantify this relationship between light (both UV and VIS), temperature, and coral bleaching. In particular, Lesser (1997) found that high UV exposure can exacerbate temperature stress. Cloud cover has been implicated as mediating temperature-induced bleaching by providing shading from PAR (Mumby et al., 2001). Finally, Ferrier-Pages et al. (2007) found that prolonged UV exposure at non-stressful temperatures could protect corals from subsequent temperature-induced bleaching.
Low tides and/or low wind speeds have also been implicated as potential factors contributing to coral bleaching (Glynn, 1968; Jaap, 1979; Fisk and Done, 1985; Harriott, 1985; Oliver, 1985; Jones, 1997; Hendee et al., 2001). The former could cause bleaching by aerial exposure of corals (Vaughan, 1911; Loya, 1976) or by reducing the water thickness through which incident light must penetrate (thereby increasing light exposure at the benthos). Colored dissolved organic matter (CDOM) in the water column attenuates downwelling UV radiation (Bricaud et al., 1981; Kirk, 1994) and thus might provide protection from UV-induced bleaching (Williams and Hallock, 2004; Zepp et al., 2008; Ayoub et al., 2012). Low wind speeds could similarly increase penetration of light through reduction in water surface reflectance (Hendee et al., 2001), or through CDOM photobleaching (Moran and Zepp, 1997; Häder et al., 1998; Zepp et al., 2008; Shank et al., 2010a; 2010b). Nevertheless, it is often difficult to determine whether these factors are acting independently or synergistically with temperature stress to contribute to coral bleaching.

Satellite assessment of coral stress has focused primarily on SST (Gleeson and Strong, 1995; Strong et al., 2004; Mumby et al., 2004). The National Oceanic and Atmospheric Administration (NOAA) Coral Reef Watch (CRW) program uses degree heating weeks (DHW; Gleeson and Strong, 1995) to assess thermal stress on corals globally, whereby the duration and intensity of elevated temperatures, based on > 1 °C differences from climatology SST, is quantified over 12 weeks. The currently operational product uses global SST data and climatology with 50 km spatial resolution, while experimental products are distributed by CRW at 5 km spatial resolution (see Vega-Rodriguez et al., 2012). Furthermore, prototype 1 km resolution products have been developed for regional applications by CRW in collaboration with the University of South Florida and the Comisión Nacional para el Conocimiento y Uso de la Biodiversidad (CONABIO) in Mexico. Finally, the CRW has also developed an experimental Light Stress Damage (LSD) product. This uses a combination of SST and satellite-derived daily PAR to assess coral bleaching stress. Validation statistics of this product have not yet been reported, but the general
approach omits consideration of UV stress, as well as variation in light reaching corals due to bottom depth and spatiotemporally variable attenuation of light in the water column.

The application of remote sensing data for determination of water clarity (i.e., light penetration) in optically shallow environments like coral habitats has been hindered by lack of robust methods for correction of benthic light reflectance effects on the remote sensing reflectance (\(R_{rs}\)) measured above the surface. Recent algorithms have been developed to estimate the diffuse downwelling attenuation coefficient (\(K_d\)) for both VIS (Barnes et al., 2013) and UV (Barnes et al., 2014) in optically shallow waters of the Florida Keys region. These products allow for assessment of the light field reaching corals for the time series of Moderate Resolution Imaging Spectroradiometer (MODIS) data, which spans 2000 to the present for the MODIS sensors on NASA’s Aqua and Terra satellites. Satellite-derived SST data does not suffer from such benthic interference (e.g., Hu et al., 2009).

Here, the roles of several environmental parameters on coral bleaching were investigated, including SST, light (VIS and UV), wind speed, and tidal regime. The environmental factors identified as contributing to coral bleaching were subsequently used to develop and validate a model for prediction of coral bleaching. The Florida Keys were used as a case study for this research, from which a large dataset of coral bleaching and satellite-derived environmental parameters exist.

2. Methods

2.1. Data collection and processing

Table 1 provides a summary of the observations compiled for this study. MODIS Aqua and Terra (MODIS/A and MODIS/T, respectively) Level-1A data for the Florida Keys region (24 to 26 °N, 80 to 83 °W; see Fig. 4.1) and the years 2000 - 2012 were downloaded from the NASA Goddard Space Flight Center (GSFC; www.oceancolor.gsfc.nasa.gov). These data were processed using SeaDAS (version 6.4) with default processing parameters to derive calibrated at-sensor radiance (Level-1B). SeaDAS was then used
to create Level-2 (unmapped calibrated) products including SST, $R_{RS}$ (for the 10 visible bands), SST Quality Flags, and Level-2 Processing Flags. Due to scan mirror damage and striping, which limit the utility of the MODIS/T instrument for ocean color research (Franz et al., 2008), $R_{RS}$ products were not created from MODIS/T.

Table 1: Summary of data compiled for this study

<table>
<thead>
<tr>
<th>Product</th>
<th>Source</th>
<th>Instrument</th>
<th>Processing</th>
<th>Initial temporal resolution</th>
<th>Final temporal resolution</th>
<th>Final spatial resolution</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>SST</td>
<td>NASA GSFC</td>
<td>MODIS/A, MODIS/T</td>
<td>SeaDAS, IMAPP, Barnes and Hu (2013)</td>
<td>$\leq 4\ d^{-1}$</td>
<td>Weekly</td>
<td>1 km</td>
<td>°C</td>
</tr>
<tr>
<td>$K_d$(488)</td>
<td>NASA GSFC</td>
<td>MODIS/A</td>
<td>SeaDAS, Barnes et al. (2013)</td>
<td>$\leq 1\ d^{-1}$</td>
<td>Weekly</td>
<td>250 m</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$K_d$(380)</td>
<td>NASA GSFC</td>
<td>MODIS/A</td>
<td>SeaDAS, Barnes et al. (2014)</td>
<td>$\leq 1\ d^{-1}$</td>
<td>Weekly</td>
<td>250 m</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>PAR</td>
<td>NASA GSFC</td>
<td>MODIS/A</td>
<td></td>
<td>Monthly</td>
<td>Monthly</td>
<td>4 km</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>Ozone</td>
<td>NASA GSFC</td>
<td>TOMS</td>
<td></td>
<td>Daily</td>
<td>Weekly</td>
<td>1.00 x 1.25 degree</td>
<td>DU</td>
</tr>
<tr>
<td>MSL</td>
<td>NOAA</td>
<td>Key West Tide Gauge</td>
<td></td>
<td>Hourly</td>
<td>Monthly</td>
<td>Entire scene</td>
<td>m</td>
</tr>
<tr>
<td>Wind speed</td>
<td>CCMP &amp; NDBC</td>
<td>Scatterometers, Anemometers</td>
<td>Triangulation, Interpolation</td>
<td>Monthly, Hourly</td>
<td>Monthly</td>
<td>0.25 degree</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>Bleaching Index</td>
<td>FRRP</td>
<td>Diving surveys</td>
<td></td>
<td>Daily</td>
<td>Daily</td>
<td>20 m$^2$ transect</td>
<td>none</td>
</tr>
</tbody>
</table>

MODIS/A and MODIS/T Level-1B data were also processed using International MODIS/Atmospheric Infrared Sounder Processing Package (IMAPP, version 2.1) to create the Level-2 MOD35 product (Ackerman et al., 2008; Ackerman et al., 2010; Frey et al., 2008). The MOD35, Level-2 SST, Level-2 Processing Flags, and SST Quality Flags were all mapped to an equidistant cylindrical projection, with bounds 24 to 26 °N and 80 to 83 °W at 1 km spatial resolution. SST data were masked according to the algorithm developed by Barnes and Hu (2013), which uses a combination of the SST Quality Flags, Level-2 Processing Flags, MOD35, temporal consistency, and difference from climatology.
SST pixels determined to be cloudy were removed from further analysis, and the mapped data were stored in Hierarchical Data Format 4 (HDF4) files.

Figure 4.1: Map of study region, indicating water depth from USGS bathymetry. Locations of FRRP and AGRRA surveys overlaid in green and red, respectively.

$R_{rs}$ data were mapped using SeaDAS to an equidistant cylindrical projection with the same bounds as for SST, but at 250 m spatial resolution. For most bands, this spatial resolution is achieved by SeaDAS via interpolation from 1 km or 500 m native pixel resolution. $R_{rs}$ data identified by any of the standard Level-2 Processing Flags (see Patt et al., 2003) were removed from further analysis. The semi-analytical algorithm developed by Barnes et al. (2013) was used to calculate $K_d(488)$ from the projected and masked $R_{rs}$ data. $K_d(380)$ was derived using the empirical orthogonal function (EOF) approach and training dataset described in Barnes et al. (2014). The minimum depth limit for application of the $K_d(488)$ and $K_d(380)$ products are 5 and 4.5 m, respectively. Any pixel with depth shallower than the respective depth limit was masked in the $K_d(380)$ and $K_d(488)$ data. Depth was determined from bathymetry
provided by the United States Geological Survey (Robbins et al., 2007). Any masked data (either due to shallow depth or Level-2 Processing Flags) surrounded by otherwise valid data were filled by linear interpolation of the adjacent pixel data. $K_d$ maps were stored in HDF4 files.

Global MODIS/A Level-3 monthly mean surface PAR data (equidistant cylindrical projection; 4km spatial resolution; Carder et al., 2003), were also downloaded from NASA GSFC. Monthly mean PAR data were used due to the higher correlation with in situ data, relative to that for satellite-derived daily (or weekly mean) PAR measurements (Frouin et al., 2012). Daily atmospheric ozone content estimates (in Dobson Units or DU) from the Total Ozone Mapping Spectrometer (TOMS) were obtained from the ancillary SeaDAS data provided by NASA GSFC (equidistant cylindrical projection; 1.00 x 1.25 degree spatial resolution). PAR and ozone data for the study region were extracted from these global images and stored as 32-bit floating points in tagged image file format (TIFF) files. Cross-Calibrated Multi-Platform (CCMP) monthly averaged ocean surface wind speed data (Level 3.5A; m s$^{-1}$; equidistant cylindrical projection; 0.25 degree spatial resolution; Atlas et al., 2010) were downloaded from NASA Physical Oceanography Distributed Active Archive Center (www.podaac.jpl.nasa.gov), and the study region data were extracted.

Tide data from the Key West tide gauge (24.555 °N, 81.807 °W) from 2002-2012 were downloaded from NOAA (www.tidesandcurrents.noaa.gov). National Data Buoy Center (NDBC) wind speed data were downloaded (www.ndbc.noaa.gov) for all buoys within the study region that had coverage spanning from 2002-2012 (FWYF1, LONF1, MLRF1, SANF1, and SMKF1). Mean sea level (MSL; m) and wind speed data at each of these stations were averaged by month and stored in ASCII text files.

Visual interpretation of the CCMP wind speed data showed incongruities for pixels adjacent to land. All pixels within approximately 0.25 degrees from land [which covers the entire Florida Reef Tract (FRT)] were masked. To fill in this area, a Delaunay triangulation was constructed to link the combined NDBC and offshore CCMP wind speed data. Linear interpolation was then used to map winds to a grid
with the same bounds as all other products and 0.25 degree spatial resolution. MLRF1 buoy data created additional errors in these combined CCMP/NDBC wind maps, and thus the interpolation was repeated excluding data from that station. These data were then used in subsequent analyses.

Weekly mean images (2002-2012) were created for all daily products [SST, $K_d(380)$, $K_d(488)$, and ozone]. Weekly mean and standard deviation climatology images were created from the weekly mean images. Monthly mean and standard deviation climatology images were created for the products with monthly resolution (PAR, wind speed, MSL). Neither diel nor day-to-day variance is accounted for in these mean, standard deviations, or climatology estimates.

The weekly / monthly mean data for the light-related products were combined to calculate measures of light reaching the benthos for both VIS and UV wavelengths. First, PAR, $K_d(488)$ and depth ($z$) were combined using Lambert-Beer’s law (Smith and Baker, 1981; Gordon, 1989) to estimate PAR at depth [hereby called ‘bottom available visible radiation’ (BAVIS)] as:

$$B\text{AV}_{\text{VIS}} \propto P\text{AR}e^{-K_d(488)z}.$$  

Next, 380 nm irradiance at the water surface [$E_d^{(380,0)}$] was approximated by:

$$E_d^{(380,0)} \propto \left[ F_0^{(380)} \left( 1 + 0.0167 \cos \left( \frac{2\pi \text{day}}{365.25} \right) \right)^2 \right] \cos \left( \frac{\text{Ozone}/1000}{\cos(\theta_o)} \right) \cos(\theta_o) \times t,$$

where $\text{day}$ is the ordinal day number (day-of-year), and $F_0$ is the mean extraterrestrial solar irradiance ($1.139 \text{ W m}^{-2} \text{ nm}^{-1}$ at 380nm; Gregg and Carder, 1990), which is corrected for Earth-Sun distance in the first bracket. $\theta_o$ is the solar zenith angle, and $t$ is the diffuse transmittance from the sun to the earth surface that can be approximated as:

$$t \approx e^{(-0.5 \tau_r / \cos(\theta_o))},$$

where $\tau_r$ is the optical thickness due to Rayleigh scattering. For an atmosphere with surface pressure of 1013.02 mbar, $\tau_r(380) = 0.4457$. Note that this calculation omits the effect of aerosol scattering because its modulation to diffuse transmittance is mostly negligible due to the fact that > 95% of scattering is in
the forward direction and diffuse transmittance due to aerosol alone is nearly 1.0. From this, the relative measure of UV light reaching the benthos [hereafter called ‘bottom available UV radiation’ (BA\textsubscript{UV})] was calculated as:

\[
BA\textsubscript{UV} \propto E_d(380,0)e^{-K_d(380)z}.
\]  

(4)

Note that terms \(BA\textsubscript{VIS}\) and \(BA\textsubscript{UV}\) explicitly refer to large spectral bands, yet these products were calculated using data from specific wavelengths. Many studies (Kratzer \textit{et al.}, 2003; Pierson \textit{et al.}, 2008; Zhao \textit{et al.}, 2012) have described a direct relationship between \(K_d\) (PAR) and either \(K_d(490)\) or euphotic zone depth [which is directly proportional to \(K_d(490)\)]. As such, although \(BA\textsubscript{VIS}\) in this study is not a direct measure of either PAR or 488 nm light at depth, it is a relative measure of PAR reaching the benthos.

The absorption spectrum of UV light in water primarily follows an exponential decay due to the absorption by CDOM (\(a_g\); Bricaud \textit{et al.}, 1981). Combined with the strong dependence of \(K_d\) (UV) on \(a_g\) (UV) (see Zepp \textit{et al.}, 2008), this means that \(K_d\) at any two UV wavelengths are directly proportional. Note that there is no atmospheric attenuation coefficient of ozone (\(K_{ozone}\)) term in the second bracket of Eq (2). This is because atmospheric ozone absorbs virtually no 380 nm light at the precision of this study (\(a_{ozone} < 0.0001 m^{-1}\)). However, \(a_{ozone}\) is much higher for other UV bands (e.g., Hartley and Huggins bands; Griggs, 1968). Since only 380 nm data is considered for Eq (2) (i.e., \(K_{ozone}\) is a constant), the calculated \(E_d(380,0)\) is appropriate as a relative measure of UV light at the water surface, influenced only by the concentration of ozone (not by the spectral differences in \(K_{ozone}\)). The subsequent \(BA\textsubscript{UV}\) product is thus representative of light reaching the benthos at any UV wavelength.

Equations (1) and (2-4) were used to create weekly maps showing the average \(BA\textsubscript{VIS}\) and \(BA\textsubscript{UV}\), respectively. Since PAR was calculated in monthly intervals, when a particular week spanned two months (e.g., the week from August 27 to September 3 in non-leap years), PAR data from the month that included at least four days of that week was used. Separate \(BA\textsubscript{UV}\) and \(BA\textsubscript{VIS}\) weekly means were also calculated after taking account of the tidal condition. This was accomplished by modifying the depth
term in Equations (1) and (4) according to MSL (i.e., \( z = \text{bathymetry} + \text{MSL} \)). Since data from only one tide gauge was used, the MSL correction was applied to the entire scene. As with the other products, weekly mean and standard deviation climatologies were created for \( \text{BA}_{\text{UV}} \) and \( \text{BA}_{\text{VIS}} \), both with and without tidal influences included. Creation of climatologies, as well as all environmental data processing, was performed using IDL (Interactive Data Language, version 8.0, Exelis Visual Information Solutions).

See Figure 4.2 for time series of all parameters from a location in the Middle Keys (24.626 N, 81.108 W).

Figure 4.2: Time series of environmental and bleaching data at a location in the Middle Keys (24.626 N, 81.108 W) from 2002 to 2013. Time series include SST (red, °C), wind speed (green, m s\(^{-1}\)), mean sea level (MSL, orange, m), ozone (black, Dobson Units), \( K_d(380) \) (purple, m\(^{-1}\)), bottom available UV radiation(\( \text{BA}_{\text{UV}}, \) Eqs. 2-4, violet, W m\(^{-2}\)), Photosynthetically Available Radiation (PAR, yellow, W m\(^{-2}\)), \( K_d(488) \) (dark blue, m\(^{-1}\)), and bottom available visible radiation (\( \text{BA}_{\text{VIS}}, \) Eq. 1, light blue, W m\(^{-2}\)). FRRP bleaching surveys denoted with black arrows, with bleaching index listed to the left.
Finally, degree heating weeks (DHW) images were created in order to assess the performance of the current CRW methodology. As such, monthly mean SST images were created using the MODIS climatology (2000 – 2012), from which the maximum monthly mean (MMM) for all pixels in the scene was calculated. For each week, DHW images were calculated as the 12 week running total of all anomalies > 1 °C above the MMM. This product is hereby termed ‘DHW*’ to differentiate it from the DHW product currently used by CRW.

2.2. In situ data

The Florida Reef Resilience Program (FRRP) has conducted surveys of coral reef environments throughout the Florida Keys since 2005 (Fig. 4.1). Every year during times of peak thermal stress (defined as summer high water temperature and maximal irradiance), locations throughout the FRT were selected according to a randomized sampling design. ‘Summer’ records span the months of August to October, while most ‘winter’ surveys were conducted in January or February. At each location, Scleractinian coral (≥ 0.4 cm diameter) size, mortality, bleaching, and disease prevalence were surveyed along two haphazardly placed 10 x 1 m belt transects (Wagner et al., 2010). Bleaching Index (BI) for each transect was calculated based on the severity of coral tissue discoloration, whereby coral colonies were allocated to one of 6 categories ranging from no bleaching ($c_1$) to completely bleached ($c_6$):

$$ BI = \frac{(c_2 + 2c_3 + 3c_4 + 4c_5 + 5c_6)}{5}, $$

where $c$ is the percentage of corals in each of the 6 bleaching categories (see Gleason, 1993; McClanahan, 2004; Edmunds et al., 2003; McClanahan et al., 2005). Metadata for the FRRP dataset indicates that BI ranges from zero (no bleaching) to 3 (all corals bleached). This contrasts with the traditional designation of BI, which can range from 0 to 1 (or 100%; see McClanahan et al., 2005). As such, FRRP BI was divided by 3 to match other data sources. Note that BI is calculated for each transect,
from which the average and standard deviation of each survey location (consisting of two transects) were calculated. Differential bleaching severity by the various taxa was not recorded. In total, 1653 records of BI between 2005 and 2012 were obtained (Figs. 4.1 & 4.3). Figure 4.3 summarizes the monthly histogram of bleaching surveys as well as the distribution of BI from these surveys.

![Histograms showing a) sampling frequency by month, and b) frequency of bleaching index values from FRRP (black ‘+’) and AGRRA (grey ‘x’) surveys. a) The data not used in analyses were from months outside ‘summer’ and ‘winter’ designations, or lacked sufficient environmental parameters for analysis. b) NB = no bleaching, MB = Moderate Bleaching, SB = Severe Bleaching as categorical designations used for CAP.](image)

Since 1998, the Atlantic and Gulf Rapid Reef Assessment (AGRRA) has surveyed coral reef locations throughout the Caribbean. Surveys conducted in May – July 2003 covered the Lower, Middle,
and Upper Keys, while the Dry Tortugas were assessed in October 2004. In total, 60 randomly selected sites (approximately 200 m x 200 m) in the FRT were surveyed, with the bleaching status of over 4000 corals recorded as ‘not bleached,’ ‘pale,’ ‘partially bleached,’ or ‘fully bleached.’ From these data, BI of all corals (not species specific) was calculated at each site via a modification of Eq (5), using only four categories (c₁ – c₄, although c₁ is not included in BI calculations) and a denominator of 3.

2.3. Combined environmental and BI data

For each bleaching observation in the coral survey record, weekly mean, weekly mean climatology, and weekly standard deviation climatology data were extracted for SST, BA_VIS, and BA_UV. Environmental conditions were determined for the week of each individual bleaching record (t₀), as well as for the 6 preceding weeks (t₁, t₂ ... t₆). Since wind speed data were binned into monthly intervals, the month and preceding month of each bleaching record were similarly extracted. Normalized anomalies for all of these data were created as \([(\text{mean} – \text{mean climatology}) / \text{standard deviation climatology}]\). The mean normalized anomaly for six weeks (t₀ to t₅) was calculated for SST, BA_UV, and BA_VIS, and for the two months of wind speed data preceding and matching each bleaching record. Finally, the weekly changes in BA_UV and BA_VIS (Δ) were calculated for six weeks (t₀ to t₅) as the difference between mean benthic available radiation during one week minus that of the previous week (e.g., Δt₂ = t₂ – t₁).

2.4. Statistical analyses

All statistical analyses were performed using Matlab (version 2011a, Mathworks). Analyses were conducted independently for summer and winter bleaching records. A stepwise multiple regression (SMR) was first performed to identify the environmental variables parsimoniously explaining variance in BI. Parsimony in ensured through forward selection of variables which independently and
significantly contribute to the explained variance, thereby increasing the statistical power of the regression (Gauch, 1993). Specifically, this SMR constructed a model for bleaching by sequentially adding independent variables which contributed the largest partial Fisher’s test statistic ($F$), stopping when addition of the next independent variable raised the model significance level above alpha ($\alpha = 0.05$) or the adjusted coefficient of determination ($R^2_{adj}$) over that of the full model (Blanchet et al., 2008). For this analysis, the continuous BI data from both FRRP and AGRRA were used as the dependent variable. Eight parameters and their interactions (a total of 36 independent variables) were included in the SMR, each summarizing 6 weeks (or two months) of data: mean standardized anomaly of SST, $BA_{UV}$, $BA_{VIS}$, and wind speed, as well as the minimum and maximum $\Delta BA_{UV}$ and $\Delta BA_{VIS}$. FRRP records with less than 3 weeks of data (out of 6 weeks) for any of the light variables were excluded from further analysis. Records with any missing SST or wind data for the last 6 weeks or 2 months, respectively, were excluded (see Fig. 4.3a).

The SMR was first performed using $BA_{UV}$ and $BA_{VIS}$ data which included MSL, and then was repeated with the MSL data excluded. The SMR with the lower Akaike information criterion (AIC; Akaike, 1974) value between these two models was used for further analysis.

A canonical analysis of principal coordinates (CAP; Anderson and Willis, 2003) was performed to model the effects of environmental variables on bleaching occurrence. Briefly, this procedure included a principal coordinates analysis (PCA) on the environmental data and subsequent canonical discriminant analysis (CDA) using these principal coordinate axes and the BI data. The number of principal coordinate axes used in the CDA was optimized according to the minimum misclassification error of the CAP as assessed by leave-one-out-cross validation (LOOCV). This CAP was performed using the Euclidian distance metric. For this analysis, the upper and lower quartile BI data were categorized as ‘severe bleaching’ and ‘no bleaching’ conditions, respectively, and all remaining BI data were categorized as ‘moderate bleaching.’ This categorical BI was used as the dependent variable for the CAP analysis. The
independent variables which were found to significantly (and parsimoniously) explain variance in bleaching occurrence via the SMR were used as the explanatory variables in the CAP. LOOCV was performed to assess classification success. Accuracy was calculated as the total number of successful classifications divided by the total number of data points. Classification success was calculated for each individual category as the number of correct classifications divided by the total number of classifications within that category.

3. Results

In total, 637 summertime (August to October) records fit the *a priori* qualifications for the analysis (6 weeks of SST data, 2 months of wind data, 3 of 6 weeks of data for each light parameter). When MSL data were excluded, SMR selected four variables which were parsimoniously contributing to the variance in bleaching: mean standardized anomaly of SST ($\beta = 0.14$; partial $R_{adj}^2 = 0.13$; $F = 93$; $p < 0.001$), mean standardized anomaly of $BA_{\text{VIS}}$ ($\beta = 0.14$; partial $R_{adj}^2 = 0.05$; $F = 44$; $p < 0.001$), the interaction of mean standardized anomaly of SST and that of wind ($\beta = 0.13$; partial $R_{adj}^2 = 0.03$; $F = 24$; $p < 0.001$), and the interaction between the mean standardized anomalies of SST and $BA_{\text{UV}}$ ($\beta = -0.06$; partial $R_{adj}^2 = 0.01$; $F = 7$; $p = 0.012$). All of the independent variables showed positive regression coefficients, with the exception of the interaction between SST and $BA_{\text{UV}}$. The cumulative $R_{adj}^2$ and AIC for the reduced model (including only these four predictors) were 0.22 and -1772, respectively.

The same four variables (mean standardized anomaly of SST, mean standardized anomaly of $BA_{\text{VIS}}$, the interaction of mean standardized anomaly of SST and that of wind, and the interaction between the mean standardized anomalies of SST and $BA_{\text{UV}}$) were selected by the SMR when monthly MSL data were included, with cumulative $R_{adj}^2 = 0.21$ and AIC = -1769. As such, the addition of monthly
MSL data to the $BA_{uv}$ and $BA_{vis}$ variables did not improve the SMR results. Accordingly, the variables used in the CAP procedure did not include influence of MSL.

For the CAP analysis, the optimal number of principal coordinate analysis axes was 2, with total model accuracy of 46% (Fig 4.4). Figure 4.4a depicts the spread of bleaching records along the two canonical axes, while Figure 4.4b shows the correlation vector for the input environmental vectors along the same two axes. For these representations, only the direction of the vectors relative to the distribution of points is important, not the orientation of vectors relative to the axes (i.e., positive or negative). The mean randomized classification success for the dependent variable (indicating the accuracy by chance), calculated using 1000 permutations, was 38%. As such, the CAP model was significant at $\alpha = 0.001$. The confusion matrix for LOOCV results is displayed in Table 2, with classification success for the no bleaching, moderate bleaching and severe bleaching categories of 60%, 30% and 64%, respectively.

For wintertime data, only 54 bleaching records fit the analysis qualifications. For both the MSL-included ($p = 0.12$) and MSL-excluded ($p = 0.16$) analyses, the overall SMR models (including all independent variables) were not significant. Accordingly, no variables were selected by the SMR as significantly contributing to the variance in bleaching, and no CAP was attempted for wintertime data.

Table 2: Counts for leave-one-out-cross-validation (LOOCV) of CAP model, using summertime data

<table>
<thead>
<tr>
<th>Summertime LOOCV</th>
<th>Modeled</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No Bleaching</td>
</tr>
<tr>
<td>Truth</td>
<td></td>
</tr>
<tr>
<td>No Bleaching</td>
<td>86 (60.1%)</td>
</tr>
<tr>
<td>Moderate Bleaching</td>
<td>82</td>
</tr>
<tr>
<td>Severe Bleaching</td>
<td>20</td>
</tr>
</tbody>
</table>
4. Discussion

4.1. Causes of coral bleaching

The summertime results indicate that temperature, light, and wind have individual and synergistic effects in contributing to coral bleaching. Positive regression coefficients indicate that higher
temperatures and BA\textsubscript{\text{vis}} were individually associated with increased BI. The significant effect of SST in causing coral bleaching is not novel (for reviews see Glynn, 1996; Brown, 1997; Hoegh-Guldberg, 1999; and others). SST was always the most significant predictor (highest partial $F$) in the SMR. However, SMR on this dataset unequivocally demonstrates that SST is not the only significant predictor of coral bleaching. Higher BA\textsubscript{\text{vis}} was associated with more severe bleaching, indicating increased shading in the VIS wavelengths caused lower BI, which also agrees with previous research (Lesser 1989; Lesser and Shick 1989; Lesser \textit{et al.}, 1990; Osmund 1994; Gleason and Wellington, 1995; Mumby \textit{et al.}, 2001).

Further, the significant interaction terms indicate that the effect of SST on bleaching is influenced by other environmental parameters. Unfortunately, these results do not indicate the direction of the UV or wind speed effects on the relationship between SST and BI (\textit{i.e.,} exacerbating or mitigating). However, the sign of the regression coefficient indicates at what temperature level UV and wind speed have an effect. Specifically, the significant interaction term between SST and wind data showed a positive regression coefficient, indicating that the effect of wind on bleaching increases as temperature increases (see below). Contrastingly, the negative regression coefficient for the interaction between SST and BA\textsubscript{\text{uv}} indicates a decreasing role of UV in contributing to bleaching as temperatures increase (see below).

The interaction of wind speed and SST potentially indicates a difference between satellite-derived SST and sea bottom temperature (SBT). SBT is the temperature which corals are experiencing, and can differ greatly from SST, especially in the presence of a strong thermocline. Generally, a thermocline would result in SST greater than SBT. However, due to flow of high-salinity and warm waters from Florida Bay, inverse thermoclines (cooler water above warm) have been observed in Florida Keys reef environments (Porter \textit{et al.}, 1999; McEachron \textit{et al.}, in prep), with potentially damaging effects on corals (Porter \textit{et al.}, 1999). In either case, persistent strong winds (the wind term used in this analysis reflected 6 weeks of wind speeds) could result in a fully mixed water column, meaning a smaller
difference between SBT and SST. Also, satellite radiometers measure the ocean skin (approximately 10 μm), which is generally 0.1 – 0.5 °C cooler than the waters immediately below (Schluessel et al., 1990; Murray et al., 2000). Although this bias is fairly constant (0.1 – 0.2 °C) in high wind conditions (> 6 m s⁻¹), it is much more variable when low winds persist (up to 1.5 °C; Donlon et al., 1999).

Given the wealth of literature indicating synergistic effects of SST and UV radiation (Siebeck, 1988; Gleason and Wellington, 1993; Fitt and Warner, 1995; Shick et al., 1996; Lesser, 1997, 2006; Lesser and Farrell, 2004; Williams and Hallock, 2004; Ferrier-Pages et al., 2007), the significant interaction between BA_{UV} and SST in contributing to coral bleaching was also an expected finding. This interaction indicated that at high temperatures, BA_{UV} has little effect on bleaching, but this effect increases with decreasing temperatures. This finding generally agrees with the widely held understanding of coral bleaching, that light stress will decrease the temperature threshold for bleaching (Lesser, 2006; Wooldridge, 2009).

Many of the factors used in these analyses have similar seasonal cycles (e.g., SST and PAR; see Fig. 4.2). The high spatial and temporal resolution employed in this study, however, reveals spatiotemporal variation which is not consistent across products with similar seasonal cycles (e.g., compare current SST and BA_{VIS} normalized anomalies in Fig. 4.5). Consideration of cumulative (6 week) normalized anomaly further obscures correlation between the environmental variables. For example, despite relatively high correlation between BA_{UV} and BA_{VIS} for a single week at the FRRP bleaching survey sites ($R^2 = 0.50$ for non-zero summertime data), there is low correlation between the cumulative (6 week) BA_{UV} and BA_{VIS} standardized anomaly terms used in the SMR (excluding 3 obvious outliers, $R^2 = 0.23$). This is due to the low BA_{UV} values and subsequently low standard deviation climatology of BA_{UV}. As a result, very small errors in derived BA_{UV} can greatly affect the calculated relationship between BI and BA_{UV}. It is thus possible that the significant relationship between BA_{VIS} and coral bleaching may include some influence of UV light which was obscured by the low variability in BA_{UV}. 

46
Figure 4.5: CAP-predicted satellite bleaching (satellite bleaching product, lower panel) for the week of September 24 – 30, 2005. Normalized anomaly conditions of SST, wind speed, BA$_{\text{UV}}$, and BA$_{\text{VIS}}$ shown for the current conditions (top row) and the cumulative (preceding 6 week average, center row) time spans. CAP predicted bleaching (bottom) shown with overlaid FRRP bleaching records.

Inclusion of MSL data did not improve the AIC of the SMR model, leading to the finding that no influence of tide on coral bleaching was detected in this study. Tidal range at the Key West tide gauge is generally less than 1 m (approximately 60 cm for spring tides). The range of monthly MSL throughout a year is approximately 40 cm, while interannual monthly differences in MSL during summer months are generally on the order of 10 cm (see Fig 4.2). Since the mean depth of bleaching records in the FRRP dataset is 8.1 m, the effect of MSL variations on light penetration (via changing the depth of water) to the benthos is typically negligible. For $K_d$ of 0.5 m$^{-1}$, an increase in depth from 8.1 to 8.2 m yields only a
0.08% decrease (arithmetic difference) in the percentage of light penetrating to the benthos, although this effect is much greater for shallower depths.

Also, monthly MSL from only one single station was considered in this study. Although no effect of MSL on coral bleaching was detected, potential impacts of tide on bleaching cannot be completely disregarded. Although not commonly seen for most of the FRT, low tides leading to aerial exposure of corals and subsequent bleaching have been observed in the Dry Tortugas (Vaughan, 1911). Furthermore, site-specific tide measurements at the time of bleaching records might allow for a more robust assessment of the effect of tide on coral bleaching. Finally, the effect of tide is potentially much larger for regions with a larger tidal range.

4.2. Improvement over SST and DHW for modeling bleaching

The average normalized anomaly of SST data was the most significant factor in both the SMR and the CAP. Indeed, the CAP procedure performed using only the SST data as a predictor variable produced a significant model with total accuracy of 42%. Nevertheless, BA_{VIS} and two interaction terms were statistically significant factors in the SMR, parsimoniously explaining the variance in bleaching. Furthermore, inclusion of the BA_{VIS}, WIND/SST interaction, and BA_{UV}/SST interaction terms in the CAP improved the total accuracy as well as the classification success for all of the bleaching categories (for SST-only CAP, classification success of no bleaching = 58%, moderate bleaching = 22%, and severe bleaching = 63%).

Mean normalized anomaly of SST data from \( t_0 \) to \( t_5 \) was used in this study to account for cumulative thermal stress. This metric is similar to the CRW DHW in accounting for cumulative SST anomaly data relative to the climatology for that location. However, dividing the SST anomaly by the climatology standard deviation accounts for acclimation of corals to the particular interannual
temperature regime (variable or constant) at their location. In contrast, DHW uses an arbitrary threshold of 1 °C above the climatology to quantify thermal stress.

To assess the utility of DHW in detecting coral bleaching, the analyses were repeated using only the DHW product calculated in this study (DHW*) as a predictor. As such, the SMR indicated that DHW* significantly explained variance in bleaching occurrence, although the fit of the model was reduced ($R^2_{adj} = 0.02$; $F = 13; p = 0.003$). The subsequent CAP model was not significant at $\alpha = 0.001$, with accuracy of 30%.

This result does not necessarily reflect inaccuracies in coral bleaching detections using DHW by CRW, as there are many differences between DHW* in this study and the DHW used by CRW. Specifically, DHW* products are based on the 2000-2012 SST climatology from MODIS/A and MODIS/T data. In contrast, the operational CRW climatology includes Multi-Channel Sea Surface Temperature (McClain et al., 1985) records from 1985-1993 (excluding 1991-1992 data), derived using Advanced Very High Resolution Radiometer data (Gleeson and Strong 1995; Liu et al., 2013). Both the CRW DHW and the DHW* consider 12 weeks of thermal stress, yet the former uses SST data with half-week resolution, in comparison to the coarser full-week resolution for DHW*. It is unlikely that this difference greatly affects the model results reported here. Finally, there are large differences in the spatial resolution (50 km for DHW, 1km for DHW*). As a consequence of this spatial resolution disparity, the scales of bleaching investigated by these two products are completely different. Specifically, the CRW product is designed to resolve mass bleaching events, while this study attempts detect bleaching on the approximate scale of individual reefs. Indeed, only 126 of 637 (20 %) bleaching records used in the CAP showed non-zero DHW* (bleaching is generally expected at ≥ 4 DHW; Skirving et al., 2006). Consequently, the DHW CAP model predicted ‘no bleaching’ for 80% of the bleaching records, resulting in the low overall model accuracy.
4.3. Model limitations

The concentration of zooxanthellae within corals tissues is variable due to physiological constraints or seasonal equilibrations (Fitt et al., 2001; Gleason and Wellington 1995). As such, fluctuations in zooxanthellate density can result in apparent coral bleaching, even in the absence of environmental stress (Fitt et al., 2001). Further complicating this matter, bleaching in response to environmental stress may occur much more frequently than is detected by visual surveys (Fitt et al., 2000). Indeed, using zooxanthellae counts, Fitt et al. (2000) detected widespread partial bleaching of corals (all corals sampled bleached every year for four years), yet human observers only found bleaching during two of these study years.

Beyond the uncertainties of diver-observed bleaching index, many of the model limitations stem from insufficient quantity of data in the training dataset for the CAP (i.e., the FRRP and AGRRA datasets). In particular, the FRRP dataset primarily includes bleaching data in the summertime, with only 127 bleaching records for wintertime data (collected in 2006 and 2010 only). As a result, the SMR was unable to detect any significant differences in bleaching resulting from any of the environmental parameters tested, even temperature. It is possible that bleaching observed during wintertime was residual from summer bleaching (e.g., Lang et al., 1992). Thus increasing the duration of SST stress considered may improve the model results for wintertime bleaching records. Also, mortality (not bleaching) of corals in the Florida Keys due to cold events was documented in 1962 (Shinn, 1966), 1941-1942, 1957-1958, 1963-1964, 1969-1970 (Hudson et al., 1976), 1976-1977 (Porter et al., 1982; Davis, 1982), 1981 (Walker et al., 1982), and 2010 (Lirman et al., 2011). The wintertime analyses described here would be greatly improved by inclusion of more wintertime surveys, or records of coral mortality (in addition to bleaching).

The FRRP dataset is also limited in other months, which affects the CAP-predicted bleaching results for these months. For example, AGRRA validation in 2004 was from May to July. Twenty-nine of
these ‘spring’ surveys (all but one indicating no bleaching) included sufficient satellite data for analysis using the CAP. However, the CAP misclassified all of the spring 2004 AGRRA surveys as severe bleaching. It is likely that these misclassifications would be remedied if the training dataset used for the CAP procedure included data from these spring months, however coral bleaching records during these times are scarce. Nevertheless, this result highlights the need to restrict application of this model to the months covered by the FRRP dataset (i.e., August to October).

Also, only 160 of 1652 FRRP bleaching records (130 of 1525 in summer) showed BI of 0. While this prevalence may be accurate in summer months (e.g., Fitt et al., 2000), it is unlikely that such widespread bleaching occurs in months with less thermal stress. By design, the FRRP sampling is biased towards bleaching, thus bleaching is more prevalent in the FRRP dataset than would be observed in the overall population. As a result, data in the ‘no bleaching’ category used in the CAP analysis actually includes surveys where some (albeit very slight) bleaching was observed.

Finally, the classification of BI prior to the CAP analysis is a potential source of uncertainty in the CAP results. Specifically, for this analysis, the upper and lower quartiles of BI were used to define the ‘severe bleaching’ and ‘no bleaching’ conditions, with the remaining data comprising the ‘moderate bleaching’ category. Figure 4.3a clearly shows that there are no natural breaks in the BI data to justify these particular delineations, and few surveys recorded BI greater than 0.5. As such, using different definitions of these three categories can greatly affect the accuracy and classification success of the CAP. In practice, however, several different variations of these categories (e.g., splitting the data into three equally sized groups) showed no major differences in CAP performance.

4.4. Satellite bleaching product

The LOOCV indicates high accuracy of the CAP model. LOOCV classification success of the ‘no bleaching’ and ‘severe bleaching’ data points were on the order of 3 times higher than predicted by
chance. However, classification into the ‘moderate bleaching’ category was only slightly better than chance (30% versus 25%). This result is primarily due to the lack of distinction between the ‘moderate bleaching’ category and either of the other two (see Fig. 4.3) and leads to misclassification of the ‘moderate bleaching’ records into both ‘no bleaching’ and ‘severe bleaching’ categories (see Table 2). Consequently, the classification of ‘moderate bleaching’ should be viewed with caution, and perhaps better termed ‘potential bleaching’ for prediction purposes.

As such, the CAP has been used to create maps of predicted bleaching, termed the ‘satellite bleaching product’ (SBP). Figure 4.5 shows an example SBP for the week of September 24 – 30, 2005. This map was created by extracting the SST, wind, $BA_{UV}$ and $BA_{VIS}$ data for each individual pixel for the previous 6 weeks, to create the four variables selected by the SMR as significantly contributing to bleaching. These data are then used as unknowns in a CAP procedure, whereby their PCA scores were assessed along the canonical axis and subsequently classified into one of the three bleaching categories. Overlaid on this predicted bleaching map are the FRRP records from the same week. Although the overlaid FRRP records indicate success of the SBP in predicting these bleaching events, most of the data points were included in the original LOOCV, and thus cannot be considered as a true measure of the predictive capabilities.

The wind product used in the SBP is a combination of CCMP and NOAA NDBC buoy data. The former is a reanalysis of wind data from multiple sources, and is not calculated until long after the original measurement date (currently, the CCMP dataset records do not extend past 2011). For near-real-time processing, the CCMP data could be removed from the input wind variable (leaving only NDBC data) or the wind term could be excluded from the CAP altogether. Neither of these modifications greatly diminishes the predictive capacity of the CAP. Indeed, the overall accuracy of the CAP with wind data excluded is 45%, only slightly less than the 48% accuracy the full model. This decrease in accuracy, however, results primarily from misclassification of the ‘moderate bleaching’ data (24% classification
success). The classification success was improved (compared to the full model) for both the ‘severe bleaching’ and ‘no bleaching’ categories (68% and 62%, respectively).

4.5. Future improvements

A major limitation of this work stems from a training dataset with limited temporal range which is biased towards bleaching. Additional bleaching records are required to improve both the assessment of the factors contributing to BI as well as the predictive model for bleaching. Once FRRP from 2013 are released to the public, they will provide an excellent dataset with which to assess the predictive ability of the CAP model presented here.

Also, a long-term dataset of coral bleaching in the Florida Keys has been compiled by Mote Marine Laboratory, which might be used for similar purposes. This dataset (‘BleachWatch’) is a collection of volunteer surveys, spanning June to October in each year from 2005 to the present. Each year, the FRRP uses these surveys to identify the locations and times where bleaching is potentially occurring, in order to plan subsequent FRRP surveys (Cory Walter, Mote Marine Lab, pers. comm.). As such, these data can be used to increase the number of observations (and thus the statistical power) of the SMR and CAP analyses, and further can improve the prediction of coral bleaching beyond the summertime bounds of the FRRP dataset. However, given that the BleachWatch data are a collection of volunteer surveys with non-stringent methodologies, care must be taken to assure quality control of the dataset and calibration with other data sources.

Many factors not considered in this work may also be affecting coral bleaching in the Florida Keys. In particular, the difference between SST and SBT is extremely variable in both space and time, which greatly hinders the ability to assess coral bleaching from satellite data. Current models to derive SBT from SST for Florida Keys reef environments are somewhat unreliable due to this spatial and
temporal heterogeneity. Accurate derivations of SBT from SST, however, would remove a large source of confounding error from the models presented here.

Wind direction is another parameter not considered in this study, but which might have an effect on coral bleaching in the Florida Keys. The direction of wind-driven surface currents (i.e., onshore vs. offshore) may influence the concentration of various water constituents, subsequently affecting the bottom available radiation. Although monthly mean sea level was not a significant factor in these models, it is possible that consideration of tidal level at the spatial and temporal resolution of the individual bleaching records might elucidate an effect of tide on coral bleaching. Model results might also be improved by consideration of stress on longer scales, especially for winter bleaching, which is often residual from summer bleaching events (e.g., Lang et al., 1992). Lastly, the datasets included in this study could be further supplemented with other databases (e.g., precipitation, surface currents, nutrient loadings, climactic forcings, socioeconomic status, etc.). Although inclusion of only remotely-sensed data allows for more rapid assessment of bleaching via the SBP, these other databases may improve the stepwise MLR model, and thus enhance understanding of the factors contributing to coral bleaching.

Finally, this approach must be applied to other coral environments worldwide to test its general applicability. Initially, similar analyses must be performed on regions with extensive, long-term in situ records of coral bleaching. This is imperative in order to assess whether the same factors found to be contributing to coral bleaching in the Florida Keys also are driving bleaching elsewhere. If these relationships are consistent, then the SBP can be directly applied to satellite data in coral environments worldwide, and used to identify coral bleaching potentials in near-real time. Alternatively, if the suite of environmental variables contributing to coral bleaching varies by region, then the SBP would need to be tailored to individual coral environments.
5. Conclusions

The analyses presented here quantify the relationship between coral bleaching and environmental parameters using satellite data. Elevated sea surface temperatures (SST) and high benthic available visible radiation (BA_{VIS}) parsimoniously explained variance in coral bleaching in the Florida Keys. This effect of SST was influenced by significant interactions between SST and both wind and benthic available ultraviolet radiation (BA_{UV}). Finally, the satellite bleaching product presented here represents an improvement over SST-only satellite models of coral bleaching, and allows for assessment of high-resolution coral bleaching potential over (current and historical) at weekly time scales.

6. Literature cited


Vega-Rodriguez, M., Müller-Karger, F.E., Li, J., Eakin, C.M., Guild, L., Hu, C., Lynds, S., Heron, S., Quiles-Perez, GA. (2012). Developing high-resolution thermal stress indices to enhance regional coral bleaching forecasts through NOAA’s Coral Reef Watch decision-support-system. Poster presentation, Ocean Sciences Meeting, Salt Lake City, UT, USA, 2 February 2012.


1. Introduction

When the Moderate Resolution Imaging Spectroradiometer (MODIS) time series began in 2000, coral bleaching had already been well documented (Jokiel and Coles, 1977; Glynn and D’Croz, 1990; Glynn, 1993; Brown, 1997). Indeed, one of the most widespread bleaching events in the region (and worldwide) was observed in 1998, and has been attributed to extremely high temperatures resulting from El Niño conditions (see Wilkinson, 1999). Satellite-derived sea surface temperature (SST) data from this time period is widely available, especially from the Advanced Very High Resolution Radiometer (AVHRR) instruments, which have already been used to assess coral bleaching stress (Gleeson and Strong, 1995; Strong et al., 2004; Mumby et al., 2004). Nevertheless, current AVHRR and MODIS cloud detection algorithms often fail during cold water events. Measuring the diffuse attenuation of downwelling radiation ($K_d$) in optically shallow waters using MODIS satellite data is even more technically challenging.

The work to improve satellite-based environmental data records such as SST, and $K_d$ in the visible [$K_d$(vis)] and ultraviolet [$K_d$(UV)] bands has been successful using AVHRR and MODIS measurements (Appendix A, B, C, D). These improved data records led to preliminary success in predicting coral bleaching in the study region (Chapter 4). However, climate variability has time scales of decades, and it is thus desirable to extend the present time-series analysis (2002 – 2012) to the pre-
MODIS era and also into the future. In particular, the Everglades restoration effort (Central Everglades Planning Project; US Army Corps of Engineers, 2013) is expected to alter downstream water quality, and it is critical to assess the water quality conditions along the Florida Reef Tract (FRT) using the MODIS data as baseline conditions.

Such assessments can only be achieved through the use of multiple sensors, as both MODIS instruments (onboard Terra and Aqua) are being operated well beyond their 5-year mission design. However, due to differences in spectral bands, signal-to-noise ratio, calibration, and processing algorithms, establishing multi-sensor data records for continuous water quality assessment is technically challenging. This chapter detailss some preliminary progress in this research effort, as well as discussion of future directions in forming seamless data records using modern earth-observing satellite instruments.

2. Historical perspective: the use of Landsat and SeaWiFS

The earliest multi-spectral satellite measurements of the earth’s surface were collected through the Landsat series. As such, Landsat data offer a long time series with which to assess the water quality of coastal regions at synoptic scales. This is especially necessary for the years 1986-1997, during which no ocean color satellites were in operation. However, Landsat Thematic Mapper (TM) and Enhanced Thematic Mapper (ETM+) instruments were designed mainly for land use, and therefore include fewer and wider spectral bands as well as lower signal-to-noise ratios than those designed for ocean use (Hu et al., 2012). This presents a significant challenge to establishing Landsat-based environmental data records that are consistent with those derived from modern satellite instruments such as MODIS.

To overcome this challenge, an improved atmospheric correction procedure for Landsat over ocean targets was developed based on Landsat SWIR bands, similar to the approach used for MODIS atmospheric correction. The long time series offered by Landsat TM and ETM+ were subsequently used
to derive $K_d$ over optically shallow waters in the Florida Keys, following the approach of Palandro (2006).

Briefly, for several sites within a small region where $K_d$ is expected to be the same and the sites have the same benthic type (e.g., sand) but different depths, the satellite-derived surface reflectance is an exponential function of bottom depth, and a non-linear regression can be used to derive $K_d$ for these sites. This approach was emulated for the entire time series of Landsat 5 TM data in an attempt to create 1 km synoptic maps of $K_d$ (as opposed to reef-specific estimates; Palandro, 2006). These TM estimates of $K_d$, however, showed poor correlation when compared to concurrent MODIS derivations of $K_d$ (calculated using algorithm described in Appendix C; for TM Band 1, $N = 171$; $R^2 = 0.13$). While the reasons for this divergence are still being diagnosed, it is possible that these TM derivations could be improved through use of a more accurate high resolution raster bathymetry of the Florida Keys region.

Another attempt simply used atmospherically-corrected Landsat data to examine long-term reflectance patterns, as these patterns are indicators of water quality changes. The Landsat TM reflectance data were compared with concurrent MODIS data, and results indicated that MODIS-detected remote sensing reflectance ($R_{rs}$) anomalies (2 standard deviations from monthly climatology) in the Florida Keys region were identified using Landsat data with over 90% accuracy. Historical $R_{rs}$ anomalies were then corroborated by known changes in benthic community and water clarity conditions, many of which stem from variations in local freshwater inputs to the region. The approach and the results are detailed in Appendix E – Use of Landsat data to track historical water quality changes in Florida Keys marine environments.

In contrast to Landsat TM and ETM+, the Sea-viewing Wide Field-of-view Sensor (SeaWiFS; 1997 - 2010) onboard the satellite OrbView-2 and the Coastal Zone Color Scanner (CZCS; 1978-1986) onboard Nimbus 7 both include bands which could theoretically be used for estimation of $K_d$ in optically shallow waters via the approaches described in Appendices C and D. Towards this goal, the quasi-analytical approach described in Appendix C was applied to SeaWiFS data with bounds 23 to 28°N, 76 to 84°W.
These data were compared to *in situ* $K_d$ measured in optically shallow Bahamas and Florida waters (provided by Jim Ivey, Florida Fish and Wildlife Research Institute). Unfortunately, such analysis showed poor correlation between SeaWiFS-derived $K_d$ and concurrent *in situ* data ($N = 7; R^2 = 0.0003; \text{Fig. 5.1}$).

The failure of this algorithm when applied to SeaWiFS data is likely due to differences in band centers, spectral resolution, sensor calibration, and lower signal-to-noise ratio of SeaWiFS than MODIS. While the latter may be improved by pixel binning, errors due to band center and spectral resolution differences may be ameliorated by tuning of the algorithm coefficients. In particular, NASA’s Ocean Biology Processing Group (OBPG) showed systematic difference between the MODIS $R_{rs}(667)$ and SeaWiFS $R_{rs}(670)$ in comparisons between the two instruments (see Fig. 5.2 for example comparison of MODIS and SeaWiFS $R_{rs}$). Because this is a critical band in the modified QAA algorithm (Appendix C), a tuning of the radiometric calibration may lead to improved algorithm performance.

![Figure 5.1: Comparison between concurrent and collocated *in situ* measured $K_d(490)$ and that calculated from SeaWiFS data using the approach described in Appendix C. Fill color denotes degree of temporal overlap: black = same day, grey = within 1 day, white = within 4 days. Linear trendline shown for same day matchups only.](image)

$$y = -0.002x + 0.02 \quad R^2 = 0.0003$$
3. Look into the future: Continuity of MODIS measurements

Much of the work detailed in this dissertation has focused on data from the MODIS onboard the satellite Aqua (MODIS/A). Launched in 2002, this particular instrument has already surpassed its design life (5 years) by more than 6 years. The aging of MODIS/A has led to deterioration of data quality in the blue (412 and 443 nm) bands, particularly after 2011, which has further required changes in the radiometric calibrations.

As the MODIS era winds down, the Visible Infrared Imager Radiometer Suite (VIIRS; 2011 - present) on the Suomi National Polar-orbiting Partnership satellite will continue to collect medium
resolution (~0.75 km) ocean color data. Fortunately, MODIS and VIIRS have been concurrently operational for over 2 years. This overlap is critical to allow assessment of consistency between the two sensors. As such, strong agreement of MODIS and VIIRS data products has been demonstrated for normalized water-leaving radiance and chlorophyll concentration for open ocean targets (Wang et al., 2013). Although Wang et al. (2013) noted poor VIIRS data quality for coastal environments, Hu and Le (in press) found generally consistent measures of remote sensing reflectance, chlorophyll concentration, and absorption coefficient of colored dissolved organic matter between MODIS and VIIRS in the Tampa Bay region.

Continued assessment of coral bleaching stress from satellite data requires similar work to ensure cross-sensor consistency between MODIS and VIIRS data in the Florida Keys region. An immediate step in the near future is therefore to acquire VIIRS data to develop $K_d$ (in the visible and ultraviolet wavelengths) data products, which can be subsequently evaluated against concurrent MODIS data. Once the consistency is validated, VIIRS and its successors in the coming decades will be used to establish seamless environmental data records to continue the MODIS era assessment of the water environments in the Florida Keys. Likewise, because of the wide data availability, the same approaches detailed in this dissertation may be extended to other similar shallow regions to study their long-term changes in response to climate variability and human impacts.

4. Literature cited


CHAPTER 6:
RESEARCH IMPACTS AND CONCLUSIONS

1. Summary of findings

In total, 5 existing cloud detection algorithms (one for AVHRR, four for MODIS) were found to be insufficient in differentiating clouds from valid SST measurements. Many of these deficiencies result from improper masking of valid SST during extreme cold water events. As such, two different approaches were developed that increase data quality and quantity for both AVHRR (Barnes et al., 2011) and MODIS (Barnes and Hu, 2013) SST measurements. Using these newly developed algorithms, the severity and extent of the January, 2010 cold event in Florida was quantified. AVHRR data processed using this approach were further used to assess cold temperature-induced mortality of corals in the Florida Keys (Lirman et al., 2011).

Benthic contribution to MODIS remote sensing reflectance ($R_{RS}$) was also found to cause errors in retrievals of the diffuse downwelling attenuation coefficient ($K_d$; m$^{-1}$) using existing algorithms (Zhao et al., 2013). To ameliorate this, the Quasi-Analytical Algorithm (Z. Lee et al., 2002; 2009) was modified to reduce the impact of benthic contributions (Barnes et al., 2013). The resulting optical properties were inverted to $K_d$ for all of the visible MODIS bands [$K_d$(VIS)] using the relationship described by Z. Lee et al. (2005; 2009). As such, statistically significant spatiotemporal patterns were detected, many of which agree with some aspects of previously published descriptions of regional water clarity variations (Lapointe and Clark, 1992; Szmant and Forrester, 1996; Boyer and Jones, 2002). Some of the detected patterns, however, depart from widespread perceptions of regional water clarity (specifically, higher $K_d$ in the Marquesas region than in the Middle Keys; Lapointe and Clark, 1992; Klein and Orlando, 1994;
Szmant and Forrester, 1996; Boyer and Jones, 2002), yet seem to agree with that expected from the local water circulation regime (see Smith, 1994; Porter et al., 1999; T. Lee and Williams, 1999). An algorithm to derive $K_d$ for ultraviolet (UV) wavelengths [$K_d$(UV)] was also developed for optically shallow waters in the Florida Keys (Barnes et al., 2014a). Using this approach, differences were detected between the spatial and temporal patterns of $K_d$(UV) and $K_d$(VIS) in the Florida Keys.

These algorithms were combined with other remotely sensed data sources to recreate the environmental conditions concurrent with *in situ* measures of coral bleaching. In this manner, stepwise multiple regression identified SST and benthic available visible light (BA$_{VIS}$) as factors individually (and parsimoniously) explaining variance in coral bleaching intensity. The effect of SST is further mediated by significant interactions between SST and the factors wind speed and benthic available UV radiation (BA$_{UV}$). These significant variables were subsequently used to predict coral bleaching. As such, prediction of ‘severe bleaching’ and ‘no bleaching’ conditions is achieved with 64% and 60% classification success, respectively. This predictive model outperformed similar models which use only SST data to assess coral bleaching stress (Gleeson and Strong, 1995; Strong et al., 2004; Mumby et al., 2004).

Finally, towards data continuity, attempts to directly derive $K_d$ from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) via the approach detailed in Barnes et al. (2014a) showed low correlation with concurrent and collocated *in situ* measurements. Similarly, calculations of $K_d$ from high resolution (30m) Landsat Thematic Mapper (TM) data in combination with a raster bathymetry (see Palandro, 2006) showed poor correlation with MODIS derivations. Nevertheless, after pixel binning to improve the signal-to-noise ratio, an atmospheric correction procedure was developed for TM data (similar to that used for MODIS data), from which $R_{RS}$ was calculated for TM ocean targets (Barnes et al., 2014b). TM $R_{RS}$ data were subsequently used to detect concurrent MODIS-derived $R_{RS}$ anomalies with over 90%
accuracy. As such, historical TM-detected $R_{RS}$ anomalies were used to assess long-term and spatially synoptic variations in the benthic environment and water clarity of the Florida Keys region.

2. Research implications

2.1. Coral bleaching assessment

The specific factors determined to be contributing to coral bleaching concur with many of the findings of laboratory manipulations and in situ experiments (e.g., Siebeck, 1988; Fitt and Warner, 1995; Brown, 1997; Lesser, 1997; 2006; Williams and Hallock, 2004). This agreement is despite limitations of such experiments, such as exposure of corals to unrealistic shifts in environmental parameters (e.g., Hoegh-Guldberg and Smith, 1989) and lacking temporal and spatial scope (see Hughes and Connell, 1999). Through long-term and spatially synoptic assessment of the effect of multiple factors on coral bleaching, this work supports the current perception of coral stress as being primarily temperature-induced, mediated by solar radiation (Lesser, 2006; Wooldridge, 2009), while refining the particular relationships between these stressors. The significant effects of light, both in the visible and UV wavelengths (via interaction with SST), highlight the need for assessment of both for optimal evaluation of coral bleaching stress.

The model presented for high-resolution (1km) prediction of coral bleaching from satellite data in near-real time allows for more directed response to particular bleaching events. Currently, the Florida Reef Resilience Program (FRRP) conducts its scientific surveys (i.e., standardized transects, etc.) of coral bleaching in response to bleaching reported in more informal surveys conducted by volunteers. Spatially synoptic maps of coral bleaching in near-real time could improve the planning of surveys directed to capture bleaching. Furthermore, historic assessment of coral bleaching could impact marine protected area (MPA) planning. In the Florida Keys, the Florida Keys National Marine Sanctuary conducts a re-zoning of specific protection areas every 5 years (NOAA, 2007; 2012). A long-term and
synoptic dataset of coral bleaching could direct such efforts through identification of reefs on which bleaching occurs less frequently than on nearby reefs, as well as those for which bleaching stress is a chronic issue. While it is certainly important to designate MPAs for the former (reefs where bleaching rarely occurs), protection of the latter may be even more important. For example, if healthy reefs exist in areas where bleaching is regularly expected, these corals may have acclimated to a more variable stress regime, and may thus show resilience to future stressors.

Finally, this work relies heavily on long-term databases of coral bleaching surveys in the Florida Keys. Despite the limitations of these datasets (see Chapter 4), coral environments in less affluent regions likely have fewer records of coral bleaching with less quality than those conducted in the Florida Keys. An important next step is to replicate this assessment for other areas where similar long-term databases of coral bleaching exist. If the findings presented in this study are generally applicable to other regions, then the predictive model for coral bleaching can be applied for synoptic assessment of coral bleaching of coral regions worldwide (including areas where coral bleaching has not been regularly measured). As such, both historical and ongoing (near-real time) coral bleaching can be assessed worldwide, which can have implications for MPA planning and response to severe bleaching events.

2.2. Further implications

Each of the five algorithms (two for cloud detection, three for water clarity assessment) presented in this dissertation has implications beyond use for assessment of coral bleaching. Cold events can cause detrimental effects, even leading to death, of a variety of nearshore marine organisms, including manatees (Irvine, 1983; Deutsch et al., 2003), sea turtles (Witherington and Ehrhart, 1989), fishes (Storey and Gudger, 1936; Sadovy and Eklund, 1999), mangroves (Storey and Gudger, 1936; Savage, 1972), and many others. Accurate assessment of satellite-derived SST during such events, as described in Barnes et al. (2011) and Barnes and Hu (2013), is critical to determine the extent and
severity of severe cold temperatures. Using this data, resource managers and protection agencies can better direct resources to respond to and potentially mitigate (e.g., by rescuing cold-stressed sea turtles) the damaging effects of such events.

Similarly, corals are not the only marine organisms impacted by water clarity. Seagrasses, and by extension the marine fauna that depend on them for food and/or habitat, are impacted by the light regime reaching their tissues. In particular, seagrasses experience the same photodegradation and DNA damage observed for corals (Lesser and Lewis, 1996; Zepp et al., 2008). Furthermore, seagrasses are prone to light limitation due to water column turbidity (Lapointe et al., 2004, Phipps et al., 1995) and/or epiphytization (Lapointe and Clark, 1992; Lapointe and Barile, 2004), which can cause shifts in the extent and density of seagrass environments. Seagrasses in nearby regions are generally restricted to locations where at least 20% of surface light penetrates to the benthos (Gallegos and Kenworthy, 1996), thus water clarity maps in optically shallow environments (e.g., from Barnes et al., 2013; 2014a) can be used to assess changes in the potential habitat of seagrasses as a function of light availability.

The dataset of water clarity provided using these algorithms also can serve as a baseline from which to assess the environmental impacts of major projects. In particular, the Central Everglades Planning Project (CEPP; US Army Corps of Engineers, 2013) will likely induce large alterations in the water quality of downstream ecosystems, including seagrass beds and coral reefs. Also, proposed widening of the Key West Channel to accommodate larger cruise ships will undoubtedly cause sedimentation of nearby environments. More than 10 years of MODIS data, as well as the historical perspective of water quality offered by Landsat data (Barnes et al., 2014b), comprises a platform from which the spatial scope and severity of these projects can be assessed.
3. Future work

3.1. Research directions

A major limitation of the algorithms developed to derive $K_d$ from optically shallow waters in both the UV and the VIS wavelengths is that these algorithms fail for waters shallower than a particular depth (5 m for VIS, 4.5 m for UV). As a result, no satellite water clarity data are currently obtainable for the shallowest coral environments (those receiving the largest portion of downwelling radiation). In Chapter 4, this deficiency is circumvented by extrapolation of $K_d$ from adjacent, deeper waters. This approximation, however, is not ideal, as the concentrations of various water constituents in waters overlying reefs may be influenced by adjacent land processes, resuspension due to wind and currents, or even corals themselves and associated organisms (Boss and Zaneveld, 2003). As such, more work is still needed to improve derivations of $K_d$(UV) and $K_d$(VIS) for optically shallow waters.

Future work must strive to increase the predictive capabilities of the satellite bleaching product described in Chapter 4. In particular, the prediction of coral bleaching in the Florida Keys needs to be enhanced by inclusion of more bleaching surveys into the model. The dataset of volunteer bleaching surveys collected through Mote Marine Laboratory’s BleachWatch program could be used for such a purpose. Not only would these surveys double the number of data points included in the predictive model, but the increased number of data points in non-summer months may enhance detection of coral bleaching throughout the year.

No scleractinian coral species will respond in an exactly uniform manner to physical disturbance throughout its range, and various species certainly have differential thresholds for bleaching in response to environmental stress. The results presented in this dissertation represent aggregate bleaching of coral reef communities. Where available, more robust surveys that include species-specific bleaching records (such as the Atlantic and Gulf Rapid Reef Assessment surveys), should be used to assess variations in bleaching between different coral species.
Finally, these satellite-derived databases of water parameters around coral reefs can be combined with other databases (e.g., socioeconomic, nutrient loading, climactic forcings, etc.) which may even further clarify the direct causes of coral declines. Even coarse estimates of these parameters may be useful in explaining bleaching or mortality in response to apparently low stress conditions. More accurate assessment of sea bottom temperature (SBT) from satellite-derived SST in coral environments may similarly improve model accuracy and understanding of the interactions between coral bleaching and thermal stress. In addition, the new algorithms to derive $K_d$, combined with the improvements in SST cloudmasking, may facilitate investigations of regional heat budgets (see Gramer, 2013), with implications for climate research.

3.2. Product delivery

One of the major difficulties in effective use of satellite ocean color research is dissemination of the data products in a manner that is meaningful to end-users. As potential end-users vary from resource managers to the general public, diverse methods to deliver data must be established. For example, synoptic maps of water quality, presented in near real time, may be used by researchers towards planning of scientific monitoring as well as by divers for determination of locations where the highest visibility may be expected. Similarly, near-real time maps of predicted coral bleaching should also be continually posted [akin NOAA’s current Coral Reef Watch (CRW) bleaching alerts] to identify the habitats currently at risk. As such, directed surveys of bleaching could be more effectively planned, while recreational divers could be directed to avoid stressed reef locations.

In September 2012, the $K_d$(VIS) product and subsequently determined spatiotemporal trends in Florida Keys water clarity were presented to the Water Quality Protection Program (WQPP), which advises FKNMS Sanctuary Advisory Council (SAC) on matters relating to water quality in the Keys. The purpose of this presentation was to inform the WQPP (and subsequently the SAC) of the potential of
satellite-derived water clarity products in providing data towards rezoning of the FKNMS protection areas (NOAA, 2007; 2012). Continued synthesis and dissemination of these new satellite products must continue in order to familiarize resource managers with the products to ensure their use in ongoing monitoring and conservation efforts.

Similarly, a virtual buoy system (VBS) to present satellite-derived coastal environmental data in time series format was developed (Hu et al., in press). While such an approach has been employed to great effect by NOAA CRW and the National Aeronautics and Space Administration (NASA) program Giovanni, this VBS presents coastal environmental parameters derived using regionally customized satellite algorithms (e.g., Barnes et al., 2013; 2014a) at weekly and monthly time scales. This delivery method allows for straightforward assessment of long-term trends as well as timely anomaly detection without the expense required for establishment of physical monitoring programs, and as such this system needs to be extended to the Florida Keys region in order to disseminate time series of water clarity.

4. Conclusions

Transitioning to a world of global automated technologies requires fully embracing the potential of satellites in assessment and monitoring of reef ecosystems. Beyond the simple benefits of fewer boat hours and less localized assessment, changing the scope of reef research by integrating satellite data will provide further insights into the interplay between corals and their environment. By providing a historic database of physical parameters and a clearer understanding of the factors leading to coral declines, my hope is that this research fosters enhanced coral monitoring as well as improvements in conservation and restoration efforts. Moving forward, the handful of large scale environmental factors considered in this research need to be supplemented by databases of other known coral stressors, as well as improved quantification of the sea bottom temperature from sea surface temperature data. As such, the
framework established in this dissertation will hopefully lead to an even more complete comprehension of coral bleaching and improved assessment capabilities.

5. Literature cited


APPENDIX A:

AN IMPROVED HIGH-RESOLUTION SST CLIMATOLOGY TO ASSESS COLD WATER EVENTS OFF FLORIDA

An Improved High-Resolution SST Climatology to Assess Cold Water Events off Florida

Brian B. Barnes, Chuanmin Hu, and Frank Muller-Karger

Abstract—Cloud filters developed for high-resolution (1-km) Advanced Very High Resolution Radiometer (AVHRR) satellite-derived sea surface temperature (SST) observations are generally inadequate to capture extreme cold events. Such events impacted shallow waters in Florida Bay and other coastal regions in January 2010 with fatal consequences for large numbers of corals and associated organisms. Raw AVHRR images were reprocessed to understand whether historical knowledge of daily and interannual SST variations could be used to derive a practical cloud-filtering technique. This approach, however, misidentified valid water temperature pixels by up to 20% of 2003 images collected during the month of January for each year between 1998 and 2010. To create an improved SST climatology, this cloud-filtering method was combined with manually delineated overlrides of falsely masked regions. During the January 2010 cold event, this climatology indicated negative SST anomalies of up to 1.6 °C in the Big Bend region and 14 °C in Florida Bay, with high spatial heterogeneity throughout. Our findings highlight the need for improved autonomous cloud-masking techniques to detect cold events in near real time.

Index Terms—Ocean temperature, satellites, sea measurements.

I. INTRODUCTION

Assessment of the synoptic temperature variability that affects marine ecosystems requires accurate measurement of sea surface temperature (SST) from satellites, including observations from sensors such as the National Oceanic and Atmospheric Administration (NOAA) Advanced Very High Resolution Radiometer (AVHRR) and the National Aeronautics and Space Administration Moderate Resolution Imaging Spectroradiometer (MODIS). The accuracy of these observations under cloud-free conditions has been validated using in situ measurements [1]–[5], but cloud contamination leads to significant negative bias in SST estimates [6], [7]. Although many algorithms exist to filter clouds from unprocessed (level 0) data [8], [9] with varying success, no method successfully removes all clouds while retaining all valid data.

A secondary (postprocessing) cloud filter has been proposed by Hu et al. [10] (hereafter termed “automated filter”) which is being implemented to autonomously remove cloud-contaminated pixels in SST images at the University of South Florida (USF). Inputs for this filter are images that have been calibrated, navigated, cloud filtered, and processed to SST using TerraScan software (version 3.2, SeaSpace Corporation) as described by Hu et al. [10] (termed “raw” images). The automated filter relies on the temporal stability and climatological regularity of SST for a given location (image pixel)—removing pixels which differ by either 2° from a three-day moving median value or 4° from the weekly climatological mean [10]. These threshold values were determined using long-term in situ temperature data collected along the Florida Keys Reef Tract, and the results were validated for the same region.

An extreme cold event affected South Florida and the Gulf of Mexico in January 2010. This event revealed that, for shallow waters close to land, valid SST data beyond the climatological threshold were mistakenly discarded as clouds by the automated filter. As the cloud filter was not designed to retain anomalies larger than 4 °C, other cold events in the past might also have been improperly masked for nearshore waters. An unintended consequence of this artifact is the generation of a positively biased SST climatology. The problem of false cloud masking would thus be exacerbated in filtering of future images.

All SST cloud-masking approaches seek to maximize cloud exclusion while retaining valid SST observations. The failure of the automated filter to detect the January 2010 cold event required a manual retrospective assessment of the filter performance and subsequent analysis of the climatology errors. Accurate SST assessment is crucial, as physiological deficiencies and even mortality have been reported in response to cold SST for a variety of resident organisms including corals [11], [12], manatees [13], [14], sea turtles [15], manatees [16], [17], and fishes [16], [18]. Apart from being critical to ecosystem health overall, each of these species contributes economic benefits to the State of Florida. Knowledge of extent and severity of extreme-temperature events is required to effectively monitor this coastal ecosystem and may help direct real-time research or rescue efforts. Our objective was thus to develop an improved high-resolution SST climatology to study cold events around Florida.

II. METHODS

In response to the cold event in January 2010, existing SST climatology and individual cloud-filtered images for the month of January (1995–2010) from the USF AVHRR ground station and data archive were examined. We extracted all images collected for each January from 1995 to 2010 covering waters...
around Florida (24° to 31° N, 79° to 86° W), representing a database of 3200 satellite images. Passes where the swath measured less than approximately 25% of the coverage area were discarded, leaving 2703 images.

Raw SST images processed with TeraScan to SST but not filtered using the secondary cloud-screening algorithm of Hu et al. [10] were first visually compared side by side to corresponding postprocessing filtered images [Fig. 1(a) and (b)]. Where it was apparent that the filtered image was falsely masking valid SST data, the raw image was set aside for reprocessing. This determination of valid data was based on integration of spatial and temporal information. Specifically, improper masking was documented only when the automated cloud filter removed a region-wide (approximately 200 km² or more) feature which persisted in three or more consecutive images and displayed smooth spatial gradients consistent with that expected from the underlying bathymetry and water flow regime.

The selected raw images were loaded into IDL/ENVI (version 4.5; Research Systems, Inc.) image processing software, and a region of interest (ROI) outlining the falsely masked pixels was manually created using ENVI’s ROI tool [Fig. 1(c)]. Raw data pixels covered by the ROI were passed through the automated filter to generate a new image. Those pixels outside the ROI were superimposed on the new image without modification [Fig. 1(d)]. In the creation of the ROIs, special attention was given to coastal locations as these are more likely to show faster and stronger temperature fluctuations in response to atmospheric weather patterns. In this way, the resulting filter (hereafter termed “hybrid filter”) retained the pixels deemed valid from both the raw and automatically filtered images, maximizing the amount of valid data in the image. Although this method might introduce a small degree of subjectivity, interpretation from different analyzers showed excellent consistency in identifying the misclassified pixels. Note that this manual effort was not to manually delineate clouded or mixed pixels but instead only to define a crude ROI with which to override the automated filter.

Two sets of monthly and weekly climatologies were created for January 1995–2010. The first was constructed using only the images processed with the automated filter (i.e., including those with false cloud-masking artifacts). The second climatology used the hybrid-filtered images and those images in the series with no artifacts detected. The difference between the two weekly climatologies was calculated by subtracting the first (automated) from the second (hybrid; Fig. 2). Finally, the reprocessed images and new climatologies were used to assess the extent and severity of the January 2010 cold event in Florida. Daily averaged SST composites from January 10 to 14, 2010, were subtracted from the weekly climatology to create anomaly maps (Fig. 3).

To evaluate the results of the hybrid filter, images from both filters were compared to in situ data collected from the archived National Data Buoy Center (NDBC) sea temperature data. Of the 66 NDBC stations that measured water temperature within the region studied, 26 included data that matched the AVHRR data in both time and space (Fig. 4). Data from both sources were used only if the sample times were within 0.5 h. This led to 10,578 matching pairs for the automated filter and 10,900 matching pairs for the hybrid filter. Linear regressions, root-mean-square (rms) difference, and bias calculations were performed using IDL (version 7.0; ITT Visual Information Solutions).
from extreme cold events in 2001 and 2010. The automated filter regularly masked extremely cold (i.e., differing by > 4 °C from climatology) but valid SST data in nearshore waters (see Fig. 1). The incorrect masking occurred around most of Florida’s coast, particularly in the Florida Bay and Big Bend regions. Several images also showed that the automated filter occasionally incorrectly masked warm-temperature data, particularly during warm spells in January of 1997 and 2002.

The weekly climatologies created with the hybrid filter showed substantially different average SST (+1 °C to −2 °C) than the climatologies based on the automated cloud screening. The most extreme deviations were observed nearshore during the first and second weeks of January. In the first week (January 1 to 7), the original climatology showed overall higher average SST than the hybrid climatology over the entire west coast of Florida. In the Big Bend and Florida Bay regions, this new climatology was cooler by up to 2 °C. The second week of January (days 8 to 14) showed temperatures approximately 0.5 °C lower in the nearshore regions but up to 1 °C higher in some areas of central western Florida and in Florida Bay (Fig. 2(b)). Neither the third (January 15 to 21) nor the fourth (January 22 to 28) week showed any large differences between the two climatologies.

The daily SST composites created with the two filters were compared to their corresponding filtered monthly climatologies. The original automated filter misidentified most pixels located in waters shallower than 20 m as clouds during the extreme cold event on January 11–13, 2010 (Fig. 3). The images processed with the hybrid filter, however, show that the daily averaged SST in Florida Bay during this span had negative anomalies of up to 14 °C. The maximum negative anomaly for the Big Bend region was 11.6 °C. The coldest temperatures occurred on January 11, 2010, with a slight temperature increase over the next two days (Fig. 3). Unfortunately, cloud cover on January 15 and precluded regional-region-wide examination of the days immediately preceding and following these extreme-temperature days.

The automatically filtered AVHRR data had a strong positive relationship with near-surface SST observations from NDBC buoys ($r^2 = 0.896$, $n = 10.578$, linear regression slope = 0.923, and intercept = 1.753 °C; Fig. 5). The rms difference was 0.927 °C, and the bias was 0.097 °C. The hybrid filter resulted in more matching pairs and also higher accuracy statistics. The NDBC and hybrid-filtered AVHRR data showed a strong positive relationship ($r^2 = 0.911$, $n = 10.990$, slope = 0.972, intercept = 1.323 °C, rms difference = 0.925 °C, and bias = 0.084 °C; Fig. 5). The 333 additional matching pairs (range: 6.5 °C to 27.5 °C) recovered with the hybrid filter were also strongly correlated ($r^2 = 0.979$, slope = −1.005, intercept = −0.406 °C, rms difference = 0.894 °C, and bias = −0.322 °C). These comparisons demonstrate the high quality of the AVHRR SST estimates derived using the standard algorithms, which were improperly masked under unusually cold or warm conditions. The automated filter incorrectly omitted matching pairs below 10 °C and approximately 30% of those between 10 °C and 15 °C and also had more than 10% misclassifications for pixels matched at temperatures > 26 °C (Fig. 6).
The difference between climatologies computed using the different filters was not large, primarily because the inputs for the two climatologies were identical in 81.6% of the images and most of the pixels in the reprocessed images. Furthermore, the automated filter had improperly masked both warm and cold waters at specific locations, and these errors cancelled to some degree in the climatology calculations. However, without the hybrid approach, it would be impossible to understand and quantify either positive or negative errors. The effect can be clearly visualized in Fig. 5. The images processed with the hybrid filter helped to extend the range of the observed temperatures to ~6°C and improved the matchup statistics (Figs. 5 and 6), resulting in more data coverage on individual images.

Validation against NDBC data also served to justify the manual override methodology, as the additional matching pairs showed high correlation and small error. There was a minor cold bias in these data (AVHRR data colder than NDBC data) in contrast to the slight warm bias of the entire data set. The cold bias is primarily driven by a cluster of additional matching pairs between approximately 8°C and 10°C, nearly all of which are from a single location (station 41112) during the 2010 cold event. Given the high spatial heterogeneity during this time near the St. Johns River plume, these cold-biased matches possibly are artifacts of the different spatial scales of measurement (point buoy versus 1-km² pixel satellites), or they may indicate a slight calibration error at one NDBC station.

The problem of false cloud masking of cold pixels is not unique to this region [9] or to the AVHRR sensor, as it is even present in the most sophisticated MODIS observations and cloud-screening algorithms [20]. Although the visual interpretation of thousands of images appears tedious, in practice, it is feasible and represents the best approach for climatology development. The work done here manually would nevertheless be difficult to implement in an autonomous process, yet it does serve as an example in developing the most accurate high-resolution AVHRR SST climatology for coastal regions in the global ocean that may experience extreme-temperature fluctuations.

An autonomous climatology-based filter which allowed all anomalies observed in this study (up to 14°C) would clearly be insufficient to remove clouds from this system. Alternatively, lowering filter thresholds for nearshore waters (for example, by applying a bathymetry mask) or during winter months could potentially create artificial “fronts” in the climatologies at these spatial or temporal boundaries, which might further affect subsequent image processing. Given the strong correlation between the AVHRR and NDBC data, these in situ sensors could potentially be integrated into the cloud-filtering methodology. Such a system might allow autonomous overrides of falsely masked areas but would require a more extensive sensor network to be synoptically effective.

At present, the possibility of extreme temperatures in coastal waters of Florida (and similar coastal waters in the global ocean) highlights the need for improved autonomous cloud-masking methods for high-resolution satellite satellite imagery. Furthermore, for effective monitoring of environmental parameters, it is important to continue coordinated efforts to capture SST and
bottom temperatures from local in situ sensors. Such systems allow real-time validation of filtered satellite data and provide more thorough information of the thermal conditions throughout the water column.

ACKNOWLEDGMENT

The authors would like to thank the staff of the University of South Florida (USF) Institute for Marine Remote Sensing (IMaRS) for their acquisition and geonavigation of the Advanced Very High Resolution Radiometer database. The authors would also like to thank the anonymous reviewers and the many contributors within IMaRS and the USF Optical Oceanography Laboratory who helped to greatly improve this letter. The National Data Buoy Center historical temperature measurements are provided by the National Oceanic and Atmospheric Administration (available at www.ndbc.noaa.gov), and the Florida coastline layer (Fig. 4) is obtained from the Florida Fish and Wildlife Research Institute.

REFERENCES


APPENDIX B:

A HYBRID CLOUD DETECTION ALGORITHM TO IMPROVE MODIS SEA SURFACE TEMPERATURE DATA QUALITY AND COVERAGE OVER THE EASTERN GULF OF MEXICO

A Hybrid Cloud Detection Algorithm to Improve MODIS Sea Surface Temperature Data Quality and Coverage Over the Eastern Gulf of Mexico

Brian B. Barnes and Chuanmin Hu

Abstract—Cloud contamination can lead to significant biases in sea surface temperature (SST) as estimated from satellite measurements. The effectiveness of four cloud detection algorithms for the Moderate Resolution Imaging Spectroradiometer (MODIS) in retaining valid SST data and masking cloud-contaminated data was assessed for all 24/5 daytime and nighttime images during 2010 over the eastern Gulf of Mexico and including the east coast of Florida. None of the cloud detection algorithms was found to be sufficient to reliably differentiate clouds from valid SST, particularly during anomalously cold events. The strengths and weaknesses of each algorithm were identified, and a new hybrid cloud detection algorithm was developed to maximize valid data retention while excluding cloud-contaminated pixels. The hybrid algorithm was based on a decision tree, which includes a set of rules to use existing algorithms in different ways according to time and location. Comparing with > 10,000 concurrent in situ SST measurements from buoys, images processed with the hybrid algorithm showed increases in data capture and improved accuracy statistics over most existing algorithms. In particular, while keeping the same accuracy, the hybrid algorithm resulted in nearly 20% more SST retrievals than the most accurate algorithm (Quality SST) currently being used for operational processing. The increases in both data coverage and SST range should improve MODIS data products for more reliable SST retrievals in near real time, thus enhancing the ocean observing capacity to detect anomaly events and study short- and long-term SST changes in coastal environments.

Index Terms—Cloud detection, Moderate Resolution Imaging Spectroradiometer (MODIS), remote sensing, sea surface temperature.

I. INTRODUCTION

SYNOPTIC assessment of sea surface temperature (SST) from satellite measurements is an integral component of coastal ecosystem monitoring. SST is a critical parameter to study impacts of global warming on the upper ocean layer and to monitor coastal ecosystem health. Building on the heritage established by the Advanced Very High Resolution Radiometer (AVHRR) sensors from National Oceanic and Atmospheric Administration polar-orbiting satellite series, on board the National Aeronautics and Space Administration (NASA) satellites Aqua and Terra are the Moderate Resolution Imaging Spectroradiometer (MODIS) instruments. These instruments measure long-wave and midwave infrared radiation in order to estimate SST [1]–[3]. The accuracy of the MODIS-based SST estimates has been extensively validated under cloud-free conditions [3]–[6], but contamination by even thin clouds can cause biases in SST measurements [7], [8]. As such, removal of cloud-contaminated pixels from MODIS measurements is imperative for accurate SST retrievals.

Several cloud detection algorithms have been developed for MODIS measurements to identify clouds, with varying success [9]–[13]. However, false masking of valid yet anomalously cold water pixels is a pervasive problem for cloud detection algorithms, particularly in coastal areas [12], [14]. Such shallow waters can experience extreme and rapid temperature changes in response to local air temperature changes, wind, and insolation. Accurate measurement of the SST in these environments, particularly during anomalously high temperature events, is required for synoptic assessment and monitoring of resident organisms. Cold sensitivity has been reported for a variety of organisms within the Gulf of Mexico (GOM) and nearby waters, including corals [15], [16], sea turtles [17], and manatees [18], [19]. In Florida waters during January of 2010 alone, nearly 3000 cold stunned sea turtles and 151 cold-related manatee deaths were recorded by the Florida Fish and Wildlife Conservation Commission, most of which likely occurred in areas falsely masked by current autonomous AVHRR algorithms [14]. Careful examination of MODIS SST data products, after several cloud detection algorithms are applied to mask clouds, indicates similar false cloud masking during this and other anomalous events in early 2010. More recent MODIS data collected during December 2010 suggest that this problem is not unusual, as shown in Fig. 1(a)–(d). As a result, most nearshore waters are masked as clouds, preventing the detection of cold water events. The failure to accurately retain valid SST data during extreme events also creates difficulty in both studying short-term (e.g., diurnal) changes and monitoring long-term climate change-induced impacts on the coastal environments.
Given the problems encountered by the existing cloud detection algorithms and the critical need to detect and quantify anomaly events, our objective is thus to develop an improved cloud detection algorithm to mask clouds from SST images while maximizing the retention of valid SST data. This is different from developing SST retrieval algorithms focusing on atmospheric correction and regression between apparent brightness temperature and SST.

II. EXISTING CLOUD DETECTION ALGORITHMS

Four cloud detection algorithms are assessed here, three of which are MODIS data products that have been widely used by the research community.

The first algorithm is the Level-2-flag CLDICE algorithm (hereafter termed “L2 Flags”), which determines cloud or ice presence by the Rayleigh-corrected reflectance ($R_{Rc}$) at 869 nm. Image pixels associated with $R_{Rc}(869) > 0.027$ are denoted as having “cloud or ice contamination” in bit 9 (all bit descriptions are zero based) of the Level-2 processing flags [13], which is a standard data product of the MODIS data processing software SeaDAS [20].

The second algorithm is specifically developed to evaluate SST data quality, including probability of being cloudy. For each image pixel, SST quality is assessed as a value between zero (best quality) and three (complete failure in SST retrieval). Lower values indicate better SST data quality. Fifteen quality tests are performed, and the results are used to calculate this value. These quality tests include previous masks, sensor zenith angle, distance of brightness temperatures from expected brightness temperature, and difference between calculated and reference SSTs. Each quality test is associated with a minimum
quality level, whereby failure of that test means that the overall SST quality for that pixel cannot be better than the minimum quality level. For example, the minimum quality level for the previous mask quality test is three. Therefore, a pixel which failed the previous mask test (e.g., land pixel) could not have an SST quality value of less than three. Usually high reflectance at 678 nm or nonuniform brightness temperatures could further raise the minimum quality level. A pixel that passes all quality tests is given the best SST quality value of zero [10]. Following the conventions used by the ocean research community, pixels with an SST quality value greater than or equal to two were considered not valid, i.e., contaminated by clouds. This cloud detection algorithm is termed “Quality SST” in this study.

The third cloud detection algorithm has been developed by the MODIS Cloud Mask Team, and the standard MODIS data product from this algorithm is the MOD35 algorithm. The primary output of this algorithm (bits 1 and 2 of the MOD35 product) is the rating of each pixel: confidently clear (confidence > 0.99), probably clear (0.95 < confidence ≤ 0.99), probably cloudy (0.66 < confidence ≤ 0.95), and confidently cloudy (confidence ≤ 0.66). The confidence used in this rating is based on a series of threshold tests which differ depending on time of day, solar zenith angle, glint probability, and surface type (land, water, ice, snow, coast, or desert). Each test uses three threshold values to delineate confidence (using probability values from zero to one) whether a pixel is clear. Among the threshold tests used for water pixels are temperature (water pixels cannot be below freezing temperature), difference from expected temperature, and brightness temperature spectral uniformity between 8.6, 11, and 12 µm. The tests are divided into five groups based on similarity, and the final cloud mask confidence is determined from the product of the lowest test confidences from within each group. Pixels with an overall rating of “confidently clear” or “probably clear” (bit combination 1+2 has value of two or three, respectively, where bit 2 is the most significant) were considered cloud free in this analysis, and the other pixels were regarded as “cloudy” [9], [21]–[23]. This cloud detection algorithm is termed “MOD35” in this study.

Finally, a cloud detection algorithm based purely on temporal statistics has been proposed by Hu et al. [11] to remove clouds from raw SST images. The algorithm is based on the seasonal regularity and temporal stability of SST. Each pixel is evaluated against a multiyear weekly climatology. If the current SST values deviate by > 4 °C from the climatological value, the pixel is regarded as being contaminated by clouds. If this first test is passed, the SST value is further compared to the median value of all SST data at that location within the three immediately preceding and following days. If the difference is ≤ 2 °C, the pixel is regarded as cloud free. The results have been validated for the Florida Keys region within the time period of 1995–2009 and have since been applied to other regions without validation [11]. This cloud detection algorithm is termed “Median” in this study.

III. DATA SOURCE AND PROCESSING

MODIS Aqua and Terra daytime and nighttime Level-0 data from 2010 covering the eastern GOM and the east coast of Florida (22° N to 31° N, 79° W to 91° W) were obtained from the NASA Goddard Space Flight Center. The data were processed using the SeaDAS software (version 6.1), developed by the Ocean Biology Processing Group. Specifically, the Level-0 data were processed to Level-1B data (calibrated at-sensor radiance), from which the MODIS SST algorithm [5] was applied to generate Level-2 raw (i.e., not screened for clouds) SST. Also independent of SeaDAS at Level 2 were the quality control products Quality SST [13] and L2 Flags [10]. These products were georeferenced to an equidistant cylindrical (rectangular) projection. The MOD35 algorithm was also applied to Level-1B data to generate the Level-2 MOD35 product using International MODIS/Atmospheric Infrared Sounder (AIRS) Processing Package (IMAPP) version 2.1 provided by the University of Wisconsin [24]. This IMAPP version returns the MOD35 product matching MODIS collection 5, which was then georeferenced to the same rectangular projection. All these data products were stored in Hierarchical Data Format (HDF4) files.

Raw SST data and the three cloud masks were extracted from the HDF files, with the latter generated from Quality SST, L2 Flags, and MOD35 data, respectively. For Median cloud masking, all raw SST data were used to create cloud masks using the procedure described by Hu et al. [11]. The cloud masks are raster images with one for cloud and zero for noncloud at each location (image pixel). For Quality SST, pixels with quality SST values greater than or equal to two were considered as clouds. For L2 Flags, pixels with bit 10 = 1 were considered as clouds (this only applies to daytime data; for nighttime data, the L2 Flags cloud masking was inoperable). For MOD35, pixels with values zero or one were considered as clouds. A land mask and a 1-km coastline mask were subsequently applied to each image. Overall, 2125 images between January and December 2010 were investigated, each with up to four corresponding cloud masks. Throughout this discussion, pixels which were determined to be valid noncloud SST are termed “accepted” by the algorithm, while pixels under the cloud masks have been “rejected” by the algorithm. These terms make no distinction as to whether an algorithm was correct or erroneous in this determination.

IV. HYBRID CLOUD DETECTION ALGORITHM

Each SST image, with and without cloud masks overlaid, was visually examined to determine the effectiveness of the four cloud detection algorithms. The effectiveness is measured by two criteria: 1) masking as many cloudy pixels as possible and 2) retaining as many valid pixels as possible [Fig. 1(a)–(d)]. The effectiveness was referenced against the raw SST image [Fig. 1(a)], where cloudy pixels can be easily identified visually, particularly when temporally adjacent images were compared side by side (clouds move fast, while water temperature remains relatively stable).

None of the four cloud detection algorithms was satisfactory in terms of the aforementioned two criteria, particularly when all conditions were considered: winter versus nonwinter, daytime versus nighttime, and shallow versus deep ocean. False cloud masking of large SST features (approximately
### Table 1

**Strengths and Weaknesses of the Four Current Cloud Masking Algorithms for MODIS SST**

<table>
<thead>
<tr>
<th></th>
<th>Winter (December 15 to March 19)</th>
<th>Non-Winter (March 20 to December 14)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pros</strong></td>
<td>Never accepts highly anomalous (cloudy) measurements</td>
<td>Widespread rejection (masking) of valid inshore cold pixels; Often accepts cloud edge pixels</td>
</tr>
<tr>
<td><strong>Cons</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>I2 Flags [13]</strong></td>
<td>Accepts the most anomalously cold, yet valid, SST data of any method; Great around cloud edges</td>
<td><strong>DAYTIME</strong>: Occasionally accepts pixels under thin clouds <strong>NIGHTTIME</strong>: Algorithm inoperative</td>
</tr>
<tr>
<td><strong>MODIS [12]</strong></td>
<td>Great around cloud edges</td>
<td>Sight banding; Occasionally accepts pixels under clouds <strong>DAYTIME</strong>: Often masks regions 50-75 km offshore coasts of Florida <strong>NIGHTTIME</strong>: Severe masking of inshore pixels</td>
</tr>
<tr>
<td><strong>Quality SST [10]</strong></td>
<td>Accepts the fewest cloudy pixels of any method</td>
<td>Widespread rejection of valid inshore cold pixels; Overmasking around coast and cloud edges</td>
</tr>
</tbody>
</table>

100 km² or more often occurred in nearshore shallow waters [Fig. 1(a)-(d)], particularly during anomalously cold events in winter. As expected, depending on the season, time (day or night), and locations (shallow nearshore or deep offshore waters), the performances of the four cloud detection algorithms varied, and none of them performed consistently better than the others under all circumstances. Table 1 summarizes their strengths and weaknesses.

The different performances of the four cloud detection algorithms were then used to develop a set of rules, describing a method to most effectively draw on the strengths of the input algorithms. Given the higher propensity for false cloud masking over nearshore pixels, a region of interest (ROI) was created using IDL/ENVI (version 4.5; Research Systems, Inc.) to delineate nearshore regions from offshore waters [Fig. 1(f)]. Approximately 100 km from land was designated as nearshore waters, while a 25-km distance was used in the Florida Straits and Gulf Stream. Separate cloud masking rules were applied to these nearshore and offshore regions. Likewise, data collected during the winter (December 15 to spring equinox) and nonwinter time periods required separate rules, and the lack of valid I2 Flags cloud masks during nighttime necessitated specific rules for night and day passes. Specifically, the following are observed:

1) **Daytime SST pixels are valid if they are accepted by any two of the four input cloud masking algorithms. This applies to both nearshore and offshore pixels.**
2) **Nighttime pixels (nearshore and offshore) are valid if accepted by any two of the following three algorithms: Quality SST, MODIS, and Median.**
3) **Nearshore nighttime winter pixels are valid if they are less than 2 °C from the median SST at that pixel over the time period of ±4 days (if a minimum of five valid pixels exist) or if they are accepted by any two of the following: Quality SST, MODIS, and Median.**

Each raw SST image and the corresponding cloud masks were loaded into IDL (version 8.0;ITT Visual Information Solutions), and these rules were implemented to create a hybrid cloud masking algorithm, which resulted in the cloud masked image [Fig. 1(g)]. The images were processed in time series fashion, as needed for the nighttime winter results to stabilize. This was necessary as nighttime winter image processing was dependent on future images (data from ±4 days), and no other processing was affected. A schematic decision tree for the hybrid cloud masking algorithm is shown in Fig. 2.

### V. Evaluation of Algorithm Performance

#### A. Comparison to In Situ Data

The SST data, excluding those pixels identified as clouds by the cloud masking algorithms, were evaluated against in situ temperature data obtained from moored National Data Buoy Center (NDBC) buoys. The listed accuracy of the NDBC sensors is ±0.1 °C with 0.1 °C resolution. NDBC thermistors are located within the first 2 m of the water column, and they measure the integrated temperature between the surface and the instrument depth. Data were exensively quality controlled by removing any measurement that was > 2.5 °C from the average temperature of the preceding and following 12 h. In some instances, large portions of data were removed where calibration or precision errors were apparent (e.g., if station data did not follow known seasonal cycles).
1) Pass MOD35 cloud screening?
2) Pass Median (Hu) cloud screening?
3) Pass Quality SST cloud screening?
4) Pass L2 Flags cloud screening?

Fig. 2. Schematic representation of the decision tree used in the hybrid cloud masking algorithm for determining whether a pixel is cloudy or valid SST. During daytime, pixels must be accepted by any two of the four input algorithms (1) MOD35 > 1, (2) SST within the range expected by Median, (3) Quality SST < 2, and (4) \( R_{BC}(100 \text{ nm}) < 0.027 \). At night, pixels must be accepted by any two of the three available algorithms or the additional median component for nearshore winter SST.

Fig. 3. Map of the study region and NDBC stations used for SST and cloud masking validation. Local geographic features referenced in the text are indicated in blue. Bathymetry contours show depths of 20 and 100 m as labeled. (FL) Florida.

Twenty-seventy NDBC stations in the eastern GOM recorded SST data which corresponded in space (data buoy within satellite pixel) and time (within 0.5 h) with MODIS measurements (Fig. 3). Calculations of linear regression, correlation, root-mean-square (rms) difference, and bias were performed. For each cloud masking algorithm, the MODIS/NDBC matches which were accepted as noncloudy by that algorithm but rejected by all other algorithms were further identified (these are termed as ”unique” in Fig. 4). Matching pairs with biases greater than \( \pm 3 \)°C were manually reviewed. This was accomplished by overlaying the station location on the image where the high bias matchup occurred. If the matchup was on the scan edge (high satellite zenith angle) or if a georeferencing error was apparent, the matchup was discarded.

NDBC thermistor data are typically not the best data sources to validate satellite SST, owing primarily to their relatively low stated accuracy and measurement depths. More often, shipborne radiometric data sets (e.g., [25] and [26]) are used. To our knowledge, no such data were collected at the times and locations in this scene which highlighted the largest differences in algorithm performance (shallow coastal waters during cold events; Fig. 1). NDBC stations, however, are positioned to measure these locations throughout the year. Furthermore, the use of NDBC data is warranted as this analysis is an assessment of cloud detection algorithm performance—not a validation of satellite SST retrieval algorithm as it is not the scope of this work. Indeed, the SST retrieval algorithm has been extensively validated [3]–[6] and is therefore not altered in this study. Changes in statistical performance by each algorithm depend only on the inclusion or exclusion of matchups. Finally, all algorithms are assessed using the same NDBC data set, and nearly 82% of all NDBC matches were retained by three or more of the existing algorithms. As a result, inaccuracies in the NDBC data set likely affect the performance of all algorithms equally.

Typical comparisons of satellite data with \textit{in situ} measurements consider the stability of a measurement relative to neighboring pixels (e.g., the standard deviation of a \( 3 \times 3 \) pixel square). If the pixels within this square are too variable, the pixel matchup with \textit{in situ} data is not used. Beyond the spatial uniformity tests embedded in the MOD35 and Quality SST algorithms, this technique was not employed for this investigation. Inclusion of such would have removed many instances of algorithm failure over cloudy pixels, as clouds are typically
Fig. 4. Comparison between NDBC SST and MODIS SST (within 0.5 h) after applying the four cloud masking algorithms: (a) L2 Flags, (b) MODIS, (c) Median, and (d) Quality SST. The pixels that were accepted by only one cloud masking algorithm are noted as “unique” and marked “x.” The gray diagonal is a 1:1 line, while the thick black line is the line of best fit from linear regression.

Spatially heterogeneous. Furthermore, matchups removed for proximal heterogeneity remain in the satellite data and would thus affect composite or anomaly plots. By investigating single pixel matchups only, many outliers were retained in the analysis and subsequently used to assess the performance of the various algorithms. Typically, such outliers are from erroneous accepting of cloudy pixels, but occasionally, SST can be impacted by nearby “bleeding” from nearby land-based thermal infrared radiation, leading to highly biased outliers (Fig. 5). As described earlier, a 1-km coastline mask was applied to all SST data images to remove pixels from the data set.

Overall, 1,5364 NDBC measurements matched in space and time with MODIS-derived SST data (Fig. 4). As expected, high correlations were seen between NDBC measurements and MODIS data for all cloud masking algorithms (Table II). The lowest number of matching pairs was from the L2 Flags algorithm, because this algorithm was inoperable at nighttime. Selective inclusion of daytime-only data also resulted in a slight positive bias, as deviations exist between daytime and nighttime satellite SSTs due to diurnal heating of the ocean surface [27]. The highest number of matching pairs and matchups per image was from the Median cloud masking algorithm, which also showed the most negative bias relative to all the other algorithms. When combined, these statistics reveal that, although the Median algorithm is accepting the most data points, many are actually cloudy pixels which should be rejected. Few individual matchups with large biases were seen in the Median data set, and the temperature range of SST values captured was smaller than that for most other algorithms. The MOD35 algorithm also yielded a higher number of matching pairs per image, yet correlation with concurrent NDBC measurements was lower than that for all other algorithms and the rms difference was the highest observed.

The L2 Flags, Median, and MODIS cloud masking algorithms all display an approach that is slightly too lenient in accepting cloudy pixel values, as the high data coverage (matchups per image) comes at the cost of data quality (lower accuracy statistics). In contrast, the results from the Quality SST algorithm showed very high SST accuracy ($r^2$ and rms) but the fewest matchups per image (Table II and Fig. 4). Quality SST matchups also had a much smaller SST range than those for all other algorithms. Among the four input algorithms, the Quality SST method results in the best accuracy for its SST retrievals, which justifies its use in NASA MODIS SST products. Other algorithms have increased data capture (matchups) relative to Quality SST, but some of those extra matchups are cloud contaminated and should have been rejected.
TABLE II
SUMMARY STATISTICS OF THE MATCHING PAIRS ON SPACE AND TIME BETWEEN NDBC AND MODIS DATA, AS PROCESSED BY THE FIVE CLOUD MASKING ALGORITHMS DISCUSSED. RMS IS THE RMS DIFFERENCE, $r^2$ IS THE COEFFICIENT OF DETERMINATION, AND Min and Max represent the minimum and maximum NDBC temperature measurements with matching MODIS pixel. L2 Flags is imperative for nighttime data and thus has fewer matches.

<table>
<thead>
<tr>
<th>Cloudmask Algorithm</th>
<th>Matching Pairs</th>
<th>Images</th>
<th>Matchups per Image</th>
<th>$r^2$</th>
<th>Linear Regression</th>
<th>Bias (°C)</th>
<th>RMS (°C)</th>
<th>Min (°C)</th>
<th>Max (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Median (Hu)</td>
<td>13877</td>
<td>2125</td>
<td>6.53</td>
<td>0.96</td>
<td>0.93</td>
<td>1.52</td>
<td>-0.28</td>
<td>0.97</td>
<td>8.9</td>
</tr>
<tr>
<td>L2 Flags</td>
<td>5413</td>
<td>1074</td>
<td>5.04</td>
<td>0.96</td>
<td>0.92</td>
<td>1.93</td>
<td>0.07</td>
<td>1.04</td>
<td>6.7</td>
</tr>
<tr>
<td>MODIS5</td>
<td>11996</td>
<td>2125</td>
<td>5.65</td>
<td>0.95</td>
<td>0.94</td>
<td>1.43</td>
<td>-0.16</td>
<td>1.07</td>
<td>6.7</td>
</tr>
<tr>
<td>Quality SST</td>
<td>10477</td>
<td>2125</td>
<td>4.93</td>
<td>0.97</td>
<td>0.94</td>
<td>1.45</td>
<td>-0.14</td>
<td>0.86</td>
<td>11.1</td>
</tr>
<tr>
<td>Hybrid</td>
<td>12878</td>
<td>2125</td>
<td>6.06</td>
<td>0.97</td>
<td>0.94</td>
<td>1.45</td>
<td>-0.14</td>
<td>0.91</td>
<td>6.7</td>
</tr>
</tbody>
</table>

The hybrid cloud masking algorithm developed in this study, however, demonstrated that increased data capture does not have to come at the expense of data quality (Fig. 5). While retaining accuracy and precision statistics almost identical to the Quality SST matchups, hybrid matching pairs have 20% more matchups per image (Table II). While the increase in MODIS/NDBC matchups per image (1.09) from Quality SST to hybrid data may seem small, the hybrid algorithm included over 51,000 more SST pixels per image than did the Quality SST algorithm. Furthermore, the hybrid algorithm showed a higher range of SST values accepted.

Matching pairs which were accepted by only one of the four existing cloud masking algorithms are termed “unique.” In order for a pixel to be rejected by all but one algorithm, it must share some characteristics with cloud-contaminated pixels. As such, the composition of unique matchups for an algorithm highlights the performance of that algorithm over pixels with a high probability of being cloudy. A total of 2766 NDSC/MODIS matching pairs were found to be unique (Fig. 4). For each of the input algorithms, the bias of these unique matchups was much more negative than that for the data set as a whole, a result of accepting cloud-contaminated pixels. Some unique matchups captured by the L2 Flags ($n = 53, r^2 = 0.62, bias = -2.71$, and $RMS = 0.77$) and MODIS5 ($n = 564, r^2 = 0.81, bias = -1.50$, and $RMS = 2.96$) algorithms showed extreme cold biases (up to $-22°C$) resulting from erroneous accepting of pixels in the center of clouds, not on cloud edges. As expected, these SST matches unique to the Median algorithm ($n = 1055, r^2 = 0.94, bias = -0.979$, and $RMS = 1.54$) were highly correlated and not subject to capture of highly anomalous values (in the form of either cloudy or true cold events) by algorithm design. Similarly, unique Quality SST matches ($n = 124, r^2 = 0.89, bias = -1.77$, and $RMS = 2.58$) did not greatly increase the range of temperature values accepted.

The hybrid algorithm captured 366 (13.5%) of these unique matching pairs while adding 123 pairs that were not captured by the other four (Fig. 5). These matches are from the nearshore region during winter nighttime passes since the basis for acceptance by the hybrid algorithm at all other times and locations was acceptance by two of the input cloud masks. Despite the extreme deficiencies of the input algorithms in processing of nearshore regions during this time, the 489 matching points unique to, or recaptured by, the hybrid algorithm showed a high correlation ($r^2 = 0.93$), a small bias ($-0.16°C$), and a small $RMS$ (1.07°C). Similarly, removing the recaptured matches from the unique matching pairs of the four input algorithms caused a worsening of their statistics, indicating that the hybrid algorithm is recapturing unique points that are highly correlated and unbiased while masking unique pixels which are cloud contaminated.

B. Image Scale Differences in Algorithm Performance

To compare the performances of the various cloud masking algorithms in a more synoptic manner, mean monthly composite SST maps were created for images processed with the new hybrid cloud masking algorithm as well as with each of the four input algorithms. Differences between these monthly composite SST images, using the hybrid cloud masking algorithm as a reference, were then calculated. Daytime and nighttime monthly average SST composites were compared separately owing to the facts that 1) the L2 Flags algorithm was inoperative at night and 2) potentially large differences in SST exist between daytime and nighttime as a result of diurnal heating [27]. Figs. 6 and 7 show these difference images for December and July 2010, respectively.
Assuming that the hybrid cloud masking algorithm resulted in the most accurate monthly composite, negative values in the difference images indicate that the other cloud masking algorithm either erroneously accepted cloud-contaminated (cold) pixels as valid data or falsely rejected warm pixels as invalid data. Positive values indicate the opposite. As these are monthly composites, small deviations (e.g., accepting a cloudy pixel from a single image) would show either very slight anomalies or no difference at all from the reference. For the same reasons, any large or widespread differences identified in these figures show a consistent failure in cloud masking during the month-long period.

For December (and other winter months), monthly composite differences from the input cloud masking algorithms (except L2 Flags) showed large and widespread deviations from the hybrid algorithm for nearshore pixels (Fig. 6). This is the result of false cloud masking during anomalously cold water events, and the extent of such omissions is represented by the degree of the anomaly. In nighttime composites, these anomalies occasionally exceeded 4°C for Quality SST [Fig. 6(f)] and up to 3°C
Fig. 7. Difference between July 2010 monthly composite daytime and nighttime SST images processed by the hybrid cloud masking algorithm and the four individual input cloud masking algorithms: MOD35, Median, Quality SST, and L2 Flags. Negative anomalies are due to acceptance of cloud-contaminated pixels by the input algorithm, exacerbated by rejection of valid warm (Median) or sun glint (L2 Flags) pixels. Positive deviations resulted from input filters' erroneous acceptance of northeasterly warm pixels or occasional acceptance of cloud-contaminated pixels by the hybrid filter.

For daytime winter composites, offshore results from the L2 Flags and MOD35 algorithms generally showed high similarity to those from the hybrid algorithm [Fig. 5(a) and (g)]. As there were no observed instances of widespread erroneous masking of offshore water, manual investigations of the source data of the anomaly plots (i.e., pixel SST data used to create the composite averages) were performed to identify the causes of offshore anomalies. Most cold anomalies in the composite images represent acceptance of cloudy pixels as valid data. This
problem is most prevalent in the Median (Fig. 6(c)) algorithm composites (MODIS/NDBC matchups for the Median algorithm were the most negatively biased) but is present in nearly all anomaly images.

Slight warm anomalies were also common offshore during winter, particularly for composites of Quality-SST-processed images [Fig. 6(c)]. Occasionally, erroneous acceptance of a single cloud-contaminated pixel by the hybrid algorithm resulted in a reduced average monthly SST at that location in the hybrid composite. More common, however, offshore warm anomalies were the result of a trend of decreasing SST at most pixels during the month of December; the Quality SST algorithm rejected many valid data points near the end of the month, resulting in average monthly SST which was artificially inflated. Similarly, a few of the positive and negative anomalies in winter composites resulted from erroneous masking of frontal boundaries. Whereas the hybrid algorithm properly accepted data from most fronts, the MOD35 and Quality SST algorithms often masked these areas. Consequently, when a front is present (particularly the loop current boundary), MOD35 and Quality SST images are often excluding data from this highly heterogeneous period, which resulted in incorrect monthly average SST.

During a typical summer month, composite images for all four cloud masking algorithms showed slight (typically less than 0.5 °C) deviations from the hybrid algorithm (Fig. 7). Nevertheless, the basis for these anomalies can again be determined by investigating the data that comprised the monthly composite images. Scattered negative values were ubiquitous in the Median anomaly plot, primarily resulting not only from erroneous accepting of cloud edge data but also from occasional masking of the warmest summertime data [the Median algorithm removes SST data which are above the climatological threshold; Fig. 7(c)]. Both of these effects were muted at night [Fig. 7(b)]. Negative anomalies in the MOD35, Quality SST, and L2 Flags composites are also due to erroneous acceptance of cloudy pixels. For L2 Flags, this effect is exacerbated by rejection of points with high sun glint, which were found to have slightly warmer temperatures.

MOD35, Quality SST, and L2 Flags all showed slight, yet widespread, positive anomalies (compared to the hybrid composite) during summer months (Fig. 7). The majority of these positive anomalies are the result of anomalously warm SST pixels (up to 5 °C above the monthly average) seen in three separate daytime July images, which are likely due to large-amplitude diurnal heating resulting from low winds. The relatively small total number of accepted pixels in July (due to increased cloud cover and sun glint during the summer months) means that such extreme temperature events can greatly impact the monthly mean composite for a particular cloud detection algorithm. This has the largest effect on L2 Flags composites, owing to nighttime inoperability and masking of glint-contaminated pixels. In fact, removing the three anomalous images from the L2 Flags composite greatly reduced or eliminated many of the warm anomalies in question. As in winter, some positive anomalies represent erroneous acceptance of cloudy pixels in the hybrid-algorithm-processed images. This effect is exacerbated in many locations due to small numbers of valid SST during the month at that pixel, meaning that the acceptance of temperatures slightly colder than the expected temperature (potentially cloud edge) would have a large effect on the average SST.

C. Algorithm Failure Etiology

The most expansive failures of the MOD35, Quality SST, and Median cloud detection algorithms were masking of nearshore cold water regions, which resulted from the embedded comparison to reference climatologies. For clear scenes acquired during such cold events, all cloud tests embedded within each cloud detection algorithm were analyzed individually to determine which test is causing the masking failure. Specifically, during these cold events, the failure was driven by bit 14 of the Quality SST algorithm ("SST is too different from reference"). The Median algorithm failure was due to difference from climatological SST being greater than 4 °C. For MOD35, improper cold water masking was primarily due to bit 27 (cloud flag surface temperature tests: water and night land). During the daytime, the clear-sky restoral test for ocean spatial consistency (bit 25) often properly reinstated SST values. For nighttime images, however, the restoral test for did not fully override the bit-27 failures, resulting in more extensive MOD35 failures for nighttime data. The L2 Flags algorithm, which uses only $R_{\text{b}}$ at 869 nm, is unaffected by the difference from climatologically expected SST.

VI. DISCUSSION: STRENGTHS AND WEAKNESSES

We believe that all cloud detection algorithms tested here represent the start of the art for their own purposes, as each bitwise test and the corresponding threshold value are a compromise between data quality and quantity. The approach presented here is therefore not to alter the individual algorithms but to combine the strengths of all of them to improve data quantity while retaining (and often improving) data quality, as gauged by SST validation through the use of in situ measurements.

Validation of satellite-derived SST data quality against in situ measurements has usually been performed using statistics such as $r$ (difference, coefficient of determination), and regression slope and intercept, between the two data sets. High $r^2$ and low $r$ are often used as measures of high data quality of satellite-derived SST and high performance of cloud masking algorithms [11], [14]. Under these criteria, any one of the cloud masking algorithms discussed herein could be considered sufficient. However, matches between NDSC and MODIS data represent only a tiny fraction of the synoptic SST coverage of the satellite passes (less than 0.003% in this study area), and NDSC stations are not necessarily positioned to measure areas where errors in cloud masking were most frequently observed. As a result, even slight changes in the statistical results of matchups between satellite and in situ data could represent larger differences in satellite-derived synoptic SST patterns. For example, the hybrid algorithm accepted over 647 million SST data points in 2010, while the Quality SST images retained 539 million data points (a difference of more than 108 million pixels) even though the difference in the number of NDSC/MODIS matchups was only 2401. Conversely,
some major differences in algorithm performance may not be detected with such a small sampling.

Comparisons between the NDIC/MODIS matchups accepted by each algorithm (Table II) were nevertheless sufficient to identify differences in the algorithms which concur with the broad assessment of their strengths and weaknesses (Table I). All algorithms accepted some cloudy, the severity of which can be assessed by the magnitude of the negative bias (outliers in Fig. 4) as well as the negative biases and high rms for the entire data sets (Table II). The one exception is for L2 Flags, for which selective processing of only daytime data resulted in a slightly positive bias. Compared to Quality SST data, the increase in data capture by the Median, MOD35, and L2 Flags algorithms came at the cost of reduced quality. The hybrid algorithm, however, showed high data capture and data quality.

This analysis further revealed a seasonal trend in the bias values of NDIC/MODIS matchups for all algorithms, where, ideally, there should be none (Fig. 8). Retrospective assessment of NDIC/MODIS matchups prior to 2009 also showed this same seasonal trend with different magnitudes. Since data from many different NDIC sensors were compared, it is unlikely that this bias represents an error in a particular NDIC sensor. Instead, summer heating of the NDIC buoys themselves may artificially inflate the in situ measurements, causing a negative MODIS bias. Alternatively, the seasonal bias may stem from miscalibration of the MODIS instruments or MODIS SST algorithm errors (e.g., the coefficients in the multiband nonlinear regression algorithms for atmospheric correction to minimize the effects of water vapor and dust particles) or from a seasonal difference between skin SST and integrated (0–2 m depth) water temperature recordings. The latter appears unlikely, as the same trend is seen (with different magnitudes) in bias calculations for both daytime- and nighttime-only data. Theoretically, differences between integrated 0–2-m-depth water temperature and skin SST should be higher during daytime passes than at nighttime. In the absence of another source of in situ SST measurements or ground-truthed skin SST data, it is impossible to pinpoint the exact cause. Regardless of etiology, the seasonality of the MODIS SST bias does not affect the anomaly detection and trend analysis performed in this study.

The monthly composite difference plots (Figs. 6 and 7) further support the initial assessment of the strengths and weaknesses of the existing four cloud masking algorithms (Table I). This evaluation requires the assumption that the hybrid algorithm produces the most accurate SST composites. There are, undeniably, instances where cloudy pixels are included in the hybrid data set. However, the large-scale deficiencies of the four input algorithms are manifest in the composite algorithm plots (Figs. 6 and 7), giving further credibility to the initial assumption. For example, nighttime winter images were observed to have excluded nearshore cold water, which clearly resulted in large positive anomalies compared to hybrid composites. Similarly, images processed with the Median algorithm typically accepted cloud edge data. This deficiency was manifested in widespread cold anomalies of Median composites relative to hybrid composites.

Even though many of the existing cloud masking algorithms are too inclusive of cloudy pixels (i.e., treat cloudy pixels as valid data), they often do not err on the same pixels. Thus, differential strengths and weaknesses of the four existing algorithms allow for the success of the hybrid cloud masking algorithm, which requires agreement between input algorithms. A simple combination of two existing algorithms would undoubtedly reduce the number of erroneously accepted cloudy pixels but, at the same time, would exacerbate the nearshore problems whereby cold but valid SST data are erroneously masked as clouds. Thus, a decision-tree approach to combine the four existing algorithms with a median component is necessary, and the new hybrid algorithm is designed this way.

Although the median component in the hybrid cloud masking algorithm is essentially identical to that in the Median cloud masking algorithm, differences in the data inputs to these two processes result in diverse outcomes. Specifically, the Median algorithm falsely masks cold but valid SST pixels during anomalously event because all of the temporally adjacent images have also been falsely masked, meaning that there are no valid data with which to create a median. In contrast, the median component of the hybrid cloud masking algorithm is based on the improved daytime SST data, which are effectively screened by the MOD35 and, particularly, the L2 Flags algorithms. These two algorithms generally will not mask valid daytime SST data as clouds (Fig. 6), thus resulting in sufficient number of valid SST data to compute the median for cloud screening of the nighttime data.

We find the new hybrid cloud masking algorithm to be an improvement over the four existing algorithms although certainly not without artifacts. The success of the hybrid cloud masking algorithm in all scenarios (winter versus nonwinter, daytime versus nighttime, and nearshore versus offshore waters) relative to the existing algorithms warrants reprocessing of historical MODIS SST data and implementation of autonomous processing. In particular, the increased SST coverage during extreme weather events will lead to more effective monitoring and response to thermal stress on organisms of the ecosystem level. Similarly, the significantly improved SST data quality

Fig. 8. Average monthly bias (MODIS minus NDIC) of matchups between in situ and satellite measurements. Daytime and nighttime SST data from 2010 processed by the four input algorithms (L2 Flags, Quality SST, MOD35, and Median) as well as the hybrid algorithm show a strong seasonality in bias. Such seasonality is also apparent in bias data averaged from 2000 to 2009 for both the Quality SST and L2 Flags algorithms.
and coverage during nighttime should greatly facilitate studies
to investigate diurnal changes and heat budgets of the coastal
oceans.

The iterative nature of the hybrid algorithm during winter
passes obviously makes implementation of the algorithm in
near real time difficult. Unfortunately, the reliance on future
SST is required during anomalously cold events in the re-
region, as water temperatures typically drop rapidly and slowly
increase over the subsequent days. If immediate access to
nearshore cloud-removed SST in this region (and other similar
environments) is required during anomalous events, the authors
strongly suggest the use of the daytime L2 Flags algorithm as
it does not improperly mask data according to climatological
norms. However, no existing cloud detection algorithm tested
successfully differentiated cloud from valid SST for nighttime
passes, owing to the need for implementation of the hybrid
algorithm after a four-day time lag. Although the lag is not
ideal, such reprocessing regularly occurs for ocean color data,
as the most accurate ancillary ozone and meteorological data
are typically not available for days after the initial satellite pass.

The motivation of this work was to improve MODIS SST
data quality and coverage through improvements in cloud
detection techniques. However, the hybrid cloud mask can be used
for other MODIS products as well. For example, the recent de-
velopment of the MODIS floating-algae index (PAI) [28], [29]
and color index (CI) [30] data products requires an accurate
cloud detection algorithm to mask clouds while retaining all
other ocean data (including those under severe sun glint and
nearshore waters) as input of the PAI and CI algorithms. The
cloud detection algorithm developed in this study will certainly
improve these new products to enhance our ocean observing
capability. Furthermore, the hybrid cloud mask can be used to
improve comparisons to cloud detection algorithms devel-
oped for other satelliteborne instruments (e.g., [31] and [32]).

Although it is beyond the scope of this present work, we
hope that the results that have been presented will assist in
the optimization of MODIS cloud detection algorithms for coastal
applications. The hybrid algorithm was designed for the eastern
GOM, yet the variety of environments, water flow regimes,
winter–summer SST extremes, and depth ranges included in
the study area suggests that the findings from this investigation
would be applicable in other coastal systems and marginal seas.
For example, analysis of the Yellow Sea and East China Sea
using the MODIS, Quality SST, and L2 Flags cloud detection
algorithms showed problems in all of them [http://optics.
marine.usf.edu/cgi-bin/optics_data?col=YS_ECS&current=1].

While a thorough investigation is required to pinpoint the
reason, a preliminary test through image visualization suggested
that a combination of the strengths of these existing algorithms
might also work. In the GOM, nearshore areas adjacent to
riverine discharges (e.g., Mississippi River and St. Johns River),
shallow coastal regions (Big Bend region and Florida Bay),
high nearshore relief (Desoto Canyon), and rapid water
movement regions (Florida Strata) each showed marked im-
provement in SST capture with the new hybrid cloud masking
algorithm (see Fig. 4). Similarly, enhancements in cloud re-
move while retaining more valid SST data were also
observed in all offshore environments in the study area. The
implementation of a similar algorithm in other coastal ocean
regions is thus believed to improve our ability to observe short-
and long-term changes in a variety of ocean environments.

ACKNOWLEDGMENT

The in situ historical temperature data were obtained
from the National Oceanic and Atmospheric Administration
(NOAA) at [www.nodc.noaa.gov]. The operators of the in situ
stations utilized in this study include the National Data Buoy
Center, Everglades National Park, the National Ocean Service,
the Coastal-Marine Automated Network, Petrels—U.S.,
Shell International Exploration and Production, Scripps Insti-
tute of Oceanography, and the University of South Florida.
The coastline shapefiles were acquired from the NOAA
National Geophysical Data Center [33]. The bathymetry contours are
from the Fish and Wildlife Research Institute, Florida Fish
and Wildlife Conservation Commission. The authors would
like to thank the NASA Goddard Space Flight Center for
providing the Moderate Resolution Imaging Spectroradiometer
(MODIS) data, K. Strahla of the University of Wisconsin for
providing the computer codes to generate the MODIS data product,
and P. Minnett and B. Franz for their assistance in interpreting
the SST quality flags.

REFERENCES

K. L. Crancer, D. K. Clark, R. H. Evans, F. E. Hooge, H. R. Gooden,
W. M. Halsch, R. Letellier, and P. J. Minnett, "An overview of MODIS

temperature measurements from the Moderate-Resolution Imaging Spec-
trroradiometer (MODIS) on Aqua and Terra," in Proc. IEEE IGARSS,

ment and operational application of nonlinear algorithms for the measure-
ment of sea surface temperature with the NOAA polar-orbiting environmental

[4] I. Burton and A. Pearce, "Validation of GLI and other satellite-derived
sea surface temperatures using data from the Ross Sea, Antarctica, and

Algorithms: Theoretical Basis Document Version 2.0," Univ. Miami,

temperature measured by the Moderate Resolution Imaging Spectroradi-

cloud contamination of the AVHRR data record," J. Atmos. Ocean.

"Multi-channel improvements to satellite-derived global sea surface tem-

and L. E. Grantley, "Discriminating clear sky from clouds with MODIS," J.

[10] B. Franz, "Implementation of SST Processing Within the OBPX," NASA,

C. Moses, C. Y. Zhang, L. Gruner, and J. Hendee, "Building an automa-
ted integrated observing system to detect sea surface temperature anomaly

physically based cloud screening of satellite infrared imagery for
APPENDIX C:

MODIS-DERIVED SPATIOTEMPORAL WATER CLARITY PATTERNS IN OPTICALLY SHALLOW FLORIDA KEYS WATERS: A NEW APPROACH TO REMOVE BOTTOM CONTAMINATION

MODIS-derived spatiotemporal water clarity patterns in optically shallow Florida Keys waters: A new approach to remove bottom contamination

Brian B. Barnes a,*, Chuanmin Hu a, Blake A. Schaeffer b, Zhongping Lee c, David A. Palandro d,e, John C. Lehrter b

a College of Marine Science, University of South Florida, 140 7th Avenue South, St. Petersburg, FL, 33701, USA
b National Health and Environmental Effects Research Laboratory, Gulf Ecology Division, United States Environmental Protection Agency, Gulf Breeze, FL, USA
c School for the Environment, University of Massachusetts, Boston, MA, USA
d Florida Fish and Wildlife Research Institute, Florida Fish and Wildlife Conservation Commission, St. Petersburg, FL, USA
e EncorOilUpstream Research Company, Houston, TX, USA

A R T I C L E   I N F O
Article history:
Received 19 October 2012
Received in revised form 13 March 2013
Accepted 17 March 2013
Available online xxx

Keywords:
Ocean color
Optically shallow water
Water clarity

A B S T R A C T
Retrievals of water quality parameters from satellite measurements over optically shallow waters have been problematic due to bottom contamination of the signals. As a result, large errors are associated with derived water column properties. These deficiencies greatly reduce the ability to use satellites to assess the shallow water environments around coral reefs and seagrass beds. Here, a modified version of an existing algorithm is used to derive multispectral diffuse attenuation coefficients (Kd) from MODIS/Aqua measurements over optically shallow waters in the Florida Keys. Results were validated against concurrent in situ data (Kd(488)) from 0.02 to 0.20 m−1, N = 22, R2 = 0.68, Mean Ratio = 0.93, unbiased RMS = 31%, and showed significant improvements over current products when compared to the same in situ data. (N = 13, R2 = 0.37, Mean Ratio = 1.61, unbiased RMS = 50%). The modified algorithm was then applied to time series of MODIS/Aqua data over the Florida Keys (in particular, the Florida Keys Reef Tract), whereby spatial and temporal patterns of water clarity between 2002 and 2011 were elucidated. Climatologies, time series, animal images, and empirical orthogonal function analysis showed primarily nearshore-offshore gradients in water clarity and its variability, with peaks in both at the major channels draining Florida Bay. ANOVA revealed significant differences in Kd(488) along distance from shore and geographic region. Excluding the Dry Tortugas, which had the lowest climatological Kd(488), water was clearest at the northern extent of the Reef Tract. Kd(488) significantly decreased seasonally for every region along the tract. Tests over other shallow-water tropical waters such as the Belize Barrier Reef also suggested general applicability of the algorithm. As water clarity and light availability on the ocean bottom are key environmental parameters in determining the health of shallow-water plants and animals, the validated new products provide unprecedented information for assessing and monitoring of coral reef and seagrass health, and could further assist ongoing regional zoning efforts.

© 2013 Elsevier Inc. All rights reserved.

1. Introduction

For several decades, satellite ocean color measurements have offered the ability to synoptically measure water quality parameters such as water clarity, turbidity, chlorophyll-a concentrations, and many others. Instruments such as the U.S. National Aeronautics and Space Administration’s (NASA) Moderate Resolution Imaging Spectroradiometer (MODIS) onboard the satellites Aqua and Terra, and the associated algorithms developed by the ocean color community have provided a long time series of water quality data for many regions. Largely excluded from such analyses, however, have been optically shallow waters, defined here as regions where the benthos is visible from an above-water (or satellite-borne) sensor. In such environments, some of the satellite-derived remote sensing reflectance (Rrs, see Table 1 for description of symbols used in this paper) results from reflection of light off the benthos (Massie et al., 1984; Moore & Sundman, 2003). When these bottom-contaminated Rrs are fed into current water quality or water clarity algorithms, large errors in derived products can occur. Specifically, bottom contamination has been shown to result in severe overestimation of chlorophyll concentrations (Camiciaro & Carder, 2006; Gardner et al., 2005; Hu, 2008; Schaeffer et al., 2011), particulate backscattering coefficients (bvp; Carder et al., 2005), and diffuse attenuation coefficient for downwelling irradiance (Kd; Zhao et al., 2013).

The bottom contribution to satellite-measured signals is sometimes useful towards the derivation of Kd in optically shallow waters with high resolution sensors (e.g., Landsat Thematic Mapper (TM), 30 m spatial resolution). One such method involves determining the exponential
Table 1: Description of symbols.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_d$</td>
<td>Diffuse attenuation coefficient for downwelling irradiance</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$I_d(0)$</td>
<td>Downwelling irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$I_{se}(0)$</td>
<td>Subsurface downwelling irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$I_{sw}$</td>
<td>Water leaving irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$R_{rs}$</td>
<td>Remote sensing reflectance</td>
<td>sr$^{-1}$</td>
</tr>
<tr>
<td>$R_{sr}$</td>
<td>Subsurface remote sensing reflectance</td>
<td>sr$^{-1}$</td>
</tr>
<tr>
<td>$a_{oxy}$</td>
<td>Total absorption coefficient</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_{w}$</td>
<td>Absorption coefficient of pure water</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_{s}$</td>
<td>Absorption coefficient of scattering pigments</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$b_{so}$</td>
<td>Absorption coefficient of phytoplankton pigments</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$b_{w}$</td>
<td>Total backscattering coefficient</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$b_{sw}$</td>
<td>Backscattering coefficient of pure water</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$b_{s}$</td>
<td>Backscattering coefficient of suspended particles</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
<td>nm</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Solar zenith angle</td>
<td>Degrees</td>
</tr>
<tr>
<td>$z$</td>
<td>Depth</td>
<td>m</td>
</tr>
</tbody>
</table>

decay slope of water leaving irradiance ($I_{sw}$) for regions in which pixels have varying depths but the same bottom albedo (Mackenzie, 1996; Palandri et al., 2004). This procedure, however, is labor intensive and requires extensive prior knowledge of the environment, including high resolution raster bathymetry and benthic classification. Further, the required assumption that pixels used in these analyses are homogeneous with exactly the same bottom albedo is often unrealistic in complex and spatially diverse systems such as coral reefs and seagrass beds. Finally, the repeat overpass frequency for sensors with the resolution required for such work (e.g., 16 days for Landsat) is much less than that offered by ocean color satellites with lower spatial resolution (e.g., 1–2 days for Aqua at 1 km resolution), and may thus miss much of the temporal variability in water clarity. As such, although deriving $K_d$ from high resolution satellite data is sometimes feasible with intensive labor, it is operationally impractical for widespread implementation and analysis of spatiotemporal patterns in water clarity.

The nature of bottom contamination is such that within a region of optically shallow waters and homogeneous albedo, the $K_d$ signal at geometrically shallow locations will be more affected than that at deeper locations, resulting in even larger errors in derived products. The correlation between depth and bottom-contaminated $K_d$ in such environments has been exploited in the creation of bathymetries from MODIS (Hu, 2008) and TM data (Yezenga, 1981; Stumpf et al., 2003). Water clarity maps (derived from standard algorithms) of optically shallow waters, such as those around the Florida Reef Tract (FRT), show similar trends (Fig. 1). Fig. 1 shows MODIS-derived $K_d(488)$ using the Lee et al. (2005) algorithm, where changes in water clarity are clearly associated with bathymetry. This effect is also seen in the FRT region where MODIS data is processed using the default band-ratio algorithm for $K_d$ (Mueller, 2000), further highlighting the need for an improved $K_d$ algorithm for optically shallow waters.

Marine ecosystems located within optically shallow waters (e.g., coral reefs, seagrasses and sponge beds) can be greatly affected by light availability, and thus water clarity. For example, as with all organisms performing photosynthesis, zooxanthellae (algae living in symbiosis within the coral tissues) require light for chemical energy creation. However, excess radiation (especially in the ultraviolet wavelengths) can cause oxidative stress in photosynthesising marine organisms (Fayer et al., 1994; Jokiel, 1980) including corals (Fisk & Done, 1985; Hoegh-Guldberg & Jones, 1999; Laver et al., 1990). Although corals and zooxanthellae have mechanisms to mitigate the effects of such stress (Ayoub et al., 2012; Shick & Dunlap, 2002; Shick et al., 1996), it can nevertheless deteriorate the symbiotic relationship between corals and algae, especially in conjunction with elevated sea temperatures. Under extreme stress, corals will expel the zooxanthellae from their tissues, resulting in a ‘bleached’ condition, often leading to mortality of the coral polyp (see reviews by Brown, 1997; Hoegh-Guldberg, 1999; Douglas, 2003, and others). The relationship between incident radiation and stress response in corals is also wavelength dependent (Laver et al., 1996; Zippel et al., 2008), highlining the necessity for multispectral characterization of the light field reaching coral reefs. In a more general sense, decrease in water clarity are often associated with increased nutrient loading and subsequent increases in water column chlorophyll concentrations (Riley, 1976; Roche, 1989). Not only can this reduce light availability and thereby directly affect the health of both coral (e.g., Abagam et al., 2003) and seagrass (Moore & Wetzel, 2000) environments, but it can further reduce the competitive advantage of these ecosystem engineers (Hollock & Schlegel, 1988; Hemmingsen, 1998).

In the absence of reliable satellite-derived water clarity data, in situ investigations of the relationship between light and optically shallow ecosystems must rely on localized water clarity monitoring and experimentation (e.g., Fisk & Done, 1985; Gleason et al., 2006; Hoegh-Guldberg & Jones, 1999; Laver et al., 1990; Moore & Wetzel, 2000).
2. Study Area — Florida Keys and the Florida Reef Tract

The Florida Keys are a limestone archipelago located at the southern tip of Florida (Fig. 2). These islands house over 73,000 residents (US Census Bureau, 2011) and are visited by approximately 2.5 million tourists each year who generate nearly $1.2 billion dollars for the region annually. Surrounding the Florida Keys is the Florida Keys National Marine Sanctuary (FKNMS), a 9,600 km² management protected area created by the United States Congress in 1990 (Causer, 2002). Delineation of regions within the FKNMS is most commonly described according to water quality, the local circulation patterns and adjacent water masses (Klein & Orlando, 1994). Although waters within many of the FKNMS regions can be described as optically shallow at times, this work focuses solely on those waters south of the island chain. The Florida Reef Tract (FRT) is a 270 km arc of bare and patch reefs directly south and east of the Florida Keys. Coral cover within the FRT has precipitously declined over the last several decades (Andréfouët et al., 2002; Hughes, 1994; Palandri et al., 2001, 2008). These changes have been attributed to extreme temperature events (Jasp, 1985; Orman et al., 2011; Warner et al., 1999), as well as changes in water quality (Hu et al., 2003; Lapointe et al., 2004) resulting from local anthropogenic activities (Lapointe & Clark, 1992) or eustatic sources such as Florida Bay (Smith, 1994) and Mississippi River (Pele et al., 2005; Oviatt et al., 1995). Seagrass density in the region has also decreased, most often attributed to algal blooms and epiphyte buildup (Lapointe & Clark, 1992). Although chlorophyll blooms (Hu et al., 2003) and river plumes (Hu et al., 2005) can be quantified and tracked nearby coral reef and seagrass systems, errors in current algorithms due to bottom contamination prohibit quantitative satellite monitoring of the extent and fate of such events (or their impact on the benthos) as they enter optically shallow regions.

Easterly winds are typical for this region, setting up a westward current immediately south of the Lower Keys. These prevailing winds run perpendicular to the island chain (the Upper Keys, and thus do not largely contribute to nearshore currents. Instead, the proximity of the Florida Current (precursor to the Gulf Stream) to the Upper Keys leads to primarily northeastward currents in this subregion. Eddies resulting from the Florida Current also contribute to the westward flow in the Lower Keys. The Middle Keys are considered a transition zone between these two current regimes (Lee, 2012; Lee & Williams, 1998; Lee et al., 2002). General circulation patterns also show large scale (mood) of the FRT with Florida Bay waters occurring through a few channels between islands of the Florida Keys, especially Moser Channel, Long Key Channel, Channel #1 and Channel #5 (Smith, 1994; Porporo et al., 1999; Lee & Smith, 2002; Lee et al., 2002; Fig. 2). In fact, Fig. 2 appears to show increased attenuation in waters flowing into the FRT through the Middle Keys channels.

These general circulation patterns, coupled with the findings by Lapointe & Clark (1992) and Szramt & Forrester (1996) that the highest nutrient concentrations in the region were within the Middle Keys during summer months, led to the widely held hypothesis that the Middle Keys region has the lowest water clarity. Boyer and Jones (2002) found the Marquesas region to have the highest chlorophyll concentrations, while several studies have found the Lower Keys to have clearest waters (Boyer & Jones, 2002; Klein & Orlando, 1994; Szramt & Forrester, 1996). Finally, strong gradients in water quality have been identified according to distance from shore, with offshore waters being the clearest and most oligotrophic (Lapointe & Clark, 1992; Szramt & Forrester, 1996).

The Florida Bay Water Quality Monitoring Program (see Boyer & Bricenon, 2011) and the NOAA Atlantic Oceanographic and Meteorological Laboratory’s South Florida Program (see Kebbe & Bore) (2007) are long term intensive monitoring efforts in the Florida Keys region designed to investigate spatio-temporal water quality patterns. These programs provide a long term series of nutrient dynamics snapshots in the region, but are lacking in temporal resolution (>2 months) and are not spatially synoptic. Regional managers are currently planning a rezoning of specific protection areas within the FKNMS (NOAA, 2007, 2012). Synoptic water clarity information, as well as investigations of the effects of light on benthic communities, would be a timely and valuable addition to the dataset informing this process.

3. Satellite derived attenuation in optically shallow waters

3.1. Algorithm development

Among the current algorithms to derive Kd from MODIS data, Zhao et al. (2013) found that the Lee et al. (2005) algorithm (hereafter termed ‘standard Kd, Lee’2) performed better than other empirical methods when validated against concurrent in situ data from south Florida and Caribbean waters. Nevertheless, the algorithm was designed for optically deep waters, thus generally limited in its applicability for measurements contaminated by bottom reflectance. This algorithm uses a simple function to derive multispectral Kd:

\[ K_d = (1 + 0.0056a) + m_1(1 - m_2e^{a_{s}B})b, \]  

where \( a \) is the total absorption coefficient, \( b \) is the total backscattering coefficient, \( \theta \) is the sun zenith angle in air, and \( m_1, m_2, \) and \( m_3 \) are constants of 0.18, 0.52, and 108, respectively. The inherent optical properties (IOPs; \( a \) and \( b \)) and \( K_d \) are wavelength (\( \lambda \)) dependent, but wavelength notation has been omitted for simplicity. IOPs are derived using the most recent version of the Quasi-Analytic Algorithm (QAAv5;
hereafter termed ‘QAA’ developed by Lee, Z., et al. (2002, 2005). This process starts with the estimation of \( a_r \) at a reference wavelength (ref), typically 555 nm for SeaWiFS and 547 nm for MODIS:

\[
a_r(\text{ref}) = a_r(\text{ref}) + 10^{-1.146 - 1.368 \times a_r(\text{ref}) - 0.49} \frac{1}{\lambda^2},
\]

where \( a_r \) is the pure water absorption coefficient from Pope and Fry (1997) and:

\[
X = \log \left( \frac{r_b(443)}{r_b(\text{ref})} + 5 \frac{r_b(667)}{r_b(490)} + \frac{1}{r_b(667)} \right),
\]

where \( r_b \) is the underwater remote sensing reflectance, \( r_b = [R_b / (0.52 + 1.7 + R_b)] \). This \( a_r \) is then used to retrieve \( b_w \) at the reference wavelength:

\[
b_w(\text{ref}) = u(\lambda) - a_r(\text{ref}) + b_w(\lambda),
\]

where \( b_w \) is the pure water backscattering coefficient from Morel (1994), and \( u(\lambda) = [u_b / (a_r + b_w)] \) calculated from \( r_b(490) \):}

\[
u(\lambda) = \frac{1}{24a_r} \left[ g_2 + \left( g_1 \right)^2 + 4g_1r_b(490) \right]^{1/2},
\]

with coefficients \( g_1 \) and \( g_2 \) equal to 0.089 and 0.125, respectively. The value of \( b_w(\text{ref}) \) at the reference wavelength is subsequently used to derive multiscal \( b_w(\lambda) \) (Gordon & Morel, 1983; Smith & Baker, 1981) and \( a_r \):

\[
b_w(\lambda) = b_w(\text{ref}) + \left[ 1 - \frac{u(\lambda)}{u(\text{ref})} \right] b_w(\lambda),
\]

\[
a_r(\lambda) = \frac{u(\lambda) - u(\text{ref})}{u(\text{ref})} a_r(\text{ref})
\]

with

\[
Y = 2.0 \left( 1 - 1.2e^{-0.15g_2} \right).
\]

Using hyperspectral \( R_b \) data of optically shallow waters, Zhao et al. (2013) also found that \( K_b \) calculated with this process showed a large effect of bottom contamination. Since the QAA begins with estimation of \( a_r \) at a reference wavelength, any errors in this single step (Eq. 2) would be propagated throughout the QAA and into the derivaton of \( K_b \). The reference wavelength of 555 nm for SeaWiFS was originally chosen because \( a_r(555) \) is relatively stable in oceanic waters where at the same time satellite measured \( R_b \) maintains high fidelity compared to those at longer wavelengths (e.g., 670 nm), but longer wavelengths were proposed for nearshore or river plume environments (Lee, Z., et al., 2002) where higher chlorophyll or sediment concentrations cause large variations in \( a_r(555) \). Variable bottom contamination will also cause large changes in the measured \( R_b \) and subsequently derived \( a_r \), especially at shorter wavelengths. At longer wavelengths, since the attenuation coefficient due to water molecules \( (a_w) \) is much higher, less bottom contamination in the measured \( R_b \) is expected. Indeed, citing the wavelength-dependent impacts of bottom contamination, Carder et al. (2005) found improvements in satellite-derived \( b_w \) and chlorophyll-a concentration measurements using 670 nm (as opposed to 555 nm for SeaWiFS) in estuarine ratio-based algorithms for optically shallow waters in this region with depths as shallow as 2 m. For optically shallow waters deeper than 5 m, errors in these same parameters were reduced by two to three fold (Carder et al., 2005). As such, for this research we modified the QAA to use 676 nm as a reference wavelength.

To apply the QAA with 676 nm as the reference wavelength, the formula for \( a_r(\text{ref}) \) was modified from Eq. (18) in Lee, Z., et al. (2002) to:

\[
a_r(\text{ref}) = a_r(\text{ref}) + 0.07 \left( r_b(\text{ref}) \right)^{1.1},
\]

and used in place of Eqs. (2) and (3). Eqs. (4)–(8) were applied as above. The multiscal \( b_w \) and \( a_r \) were subsequently input into Eq. (1) to calculate ‘modified’ \( K_b \).

The theoretical background for this algorithm modification is modified for waters shallow and close enough that bottom contamination has an effect on the \( K_b(676) \). Even though Carder et al. (2005) showed potential improvements in water property derivations in optically shallow waters down to 2 m depth by using longer wavelengths at a reference, within that work a 5 m depth threshold was selected to minimize errors throughout the application depth range. Accordingly, the scope of data considered in this analysis is limited to waters with bottom depths deeper than 5 m. Schaeffer et al. (2011) found bottom reflectance affects satellite chlorophyll retrievals in coastal Florida waters shallower than 25 m. As such, for the purposes of this research, thresholds of 5 m and 30 m are used to delineate the shallow and deep extent of optically shallow waters within the Florida Keys ecosystem.

3.2. Sensitivity simulations

A mathematical simulation was performed to investigate differences in performance of the standard and modified \( K_b \) algorithms. First, typical ranges of \( a_r(440) \), \( a_r(490) \) and \( b_w(440) \) in the FRT region were defined from field data collected during this study. A continuous range of 0–50% of benthic albedo (at 550 nm) was used to simulate conditions for a range of benthic environments in the Florida Keys, with coarse sand (often less than 5% albedo at 550 nm) and carbonate sand (up to and exceeding 50% albedo at 550 nm) being end members (Hochberg et al., 2003; Werdell & Roesler, 2003). Using the semi-analytical model described by Lee et al. (1999), various combinations of IOPs, bottom depths, and benthic albedos were used to simulate hyperspectral \( R_b(440) \) spectra. The input IOPs were also used to calculate the ‘true’ \( K_b \) by means of Eq. (1). The \( R_b(440) \) was then fed into the QAA v5.0 and the modified QAA (and subsequently \( K_b \)) to derive standard and modified \( K_b \). Error of these algorithms was then calculated as [(simulated \( K_b \) − truth)/truth].

3.3. Satellite data

All MODIS Aqua (MODIS/A, 2002–2011) Level 0 data for the Florida Keys region were downloaded from the NASA Goddard Space Flight Center ocean color website (http://oceancolor.gsfc.nasa.gov), a total of 2281 satellite passes. The data were processed at 250 m resolution using SeaDAS (version 6.2) software and default processing parameters (Bart et al., 2001). The 250 m nm had a nominal ground resolution of 250 m while other bands at 500- and 1000-m resolutions were interpolated to 250 m. For each pass, using the standard algorithms implemented in SeaDAS. Level 2 data were created including \( R_b(440) \) and standard \( K_b \) for the MODIS bands centered at 412, 443, 469, 488, 531, 547, 555, 645, 667, and 678 nm. These products were masked using the Level 2 flags ATMF/AIR, LAND, HLT, and CLDICE (see Patt et al., 2003), then subsequently mapped to an equidistant cylindrical projection with bounds 24 to 26 N, 83 to 80 W. Hereafter, the term ‘pixel’ refers to a 250 m × 250 m data bin, which has a set latitude and longitude in this projected data frame and a spatial area of 62,500 m². All data were stored in Hierarchical Data Format 4 (HDF4) computer files.
3.5. Algorithm validation methods

Concurrent (same day and location) satellite and in situ data were compared statistically using coefficients of determination \( R^2 \), linear regression, root mean squared (RMS) percentage difference, mean ratio and standard deviation ratio. Due to error in both satellite and in situ datasets, RMS was performed on an unbiased percent difference \([\text{satellite} - \text{in situ}] / (0.5 \times \text{satellite} + 0.5 \times \text{in situ})\), hereafter termed 'URMS' and reported as a percentage (Hooker et al., 2002). The significance level (\( \alpha \)) for all statistical tests was 0.05.

3.6. Algorithm validation results

It is important to reiterate that this algorithm and all quality control procedures were developed prior to the validation shown here, and that no in situ data were used for algorithm tuning or calibration. There were 13 concurrent \( K_0(488) \) matchups between the standard \( K_0 \) Lee satellite product and in situ data (Fig. 3; range 0.02–0.20 m\(^{-1}\)). These data showed a weak, yet significant, positive relationship \( R^2 = 0.37 \), linear regression slope = 0.08 and intercept = 0.18, p-value = 0.03). Ratio statistics indicate that satellite derived \( K_0(488) \) for these data is 1.61 times the measured \( K_0(488) \) with a standard deviation ratio of 0.05 and URMS error of 50%. For comparison, the modified \( K_0 \) Lee (488) algorithm produced 22 matchups with concurrent in situ measurements of the same range (Fig. 3). The different numbers of matchups between the two satellite algorithms result from higher spatial heterogeneity in the standard \( K_0 \) Lee product, which caused more data to be discarded through the \( 3 \times 3 \) spatial homogeneity test. These matchups showed a much stronger positive relationship \( R^2 = 0.68 \), slope = 0.95, intercept = -0.002, p-value < 0.0001). The \( K_0(488) \) satellite \( K_0 \) = 0.93 \( K_0 \) (in situ), and a standard deviation ratio of 0.27. URMS was reduced from 50% to 31%.

Table 2 summarizes the matchup statistics for all bands of \( K_0 \). Due to the spatial homogeneity test of the satellite data, the number of matchups was not constant across all wavelengths, or between the standard and modified algorithms (matchups were especially reduced for the standard \( K_0 \) Lee), which was much more spatially heterogeneous than the modified \( K_0 \) Lee. To ensure a fair comparison, only in situ data which had matching satellite data from both methods (‘common’) were included in the first two panels of Table 2. The third panel includes all modified \( K_0 \) Lee matchups.

Most indices showed improved statistical relationships between satellite and in situ data when using the modified \( K_0 \) Lee in place of the standard \( K_0 \) Lee. For wavelengths shorter than 500 nm \( K_0 \) matches showed improved via increased \( R^2 \), linear regression slope closer to one and intercept closer to zero, smaller p-value, mean ratio closer to one, smaller standard deviation ratio, and smaller URMS (Table 2). For wavelengths above 600 nm, improvements in \( R^2 \) and the linear regression are not always apparent, but are seen in the mean ratio, standard deviation ratio, and URMS. Statistical measures for the remaining wavelengths (531, 547, and 555 nm) show mixed measures of performance between the standard and modified \( K_0 \) Lee. Despite improvements in the linear regression statistics, \( R^2 \) and URMS were generally not improved by the modified \( K_0 \) Lee at these wavelengths.

3.7. Discussion of validation results

As demonstrated in Fig. 1, co-occurring variations in bottom depth and satellite-derived water parameters may indicate bottom contamination. The main sources of nutrients into the FRT region are the Florida Keys themselves and the channels between islands carrying Florida Bay water (Lapointe & Clark, 1992). Higher \( K_0 \) values are expected nearest these nutrient sources or in contiguous plumes extending from them. Monthly climatologies of \( K_0(488) \) derived using the standard \( K_0 \) Lee algorithm, however, show a different pattern (see Fig. 1 showing February climatology as an example). Overlaid with
bathymetric contour lines, increases in $K_d(488)$ tend to co-occur with bottom depth even away from the land. Such visualizations reiterate the problem with current algorithms, i.e. modeled parameters vary with bottom depth, and thus represent the intensity of bottom contribution to the $R_{sl}$ signal and subsequent contamination in the derived water quality parameters.

In contrast, the exact same $R_{sl}$ data were used in the creation of Fig. 4, instead processed using the modified $K_d$ Lee algorithm. With the exception of data within the 4 m contour line, the main variation in water clarity appears to be along an onshore-offshore gradient, regardless of water depth. This visualization expands the argument of improvement in water clarity derivations using the modified $K_d$ Lee(488) beyond that offered by the limited number of matchups with in situ data. However, such maps also clearly show the failure of the modified $K_d$ Lee(488) at very shallow (less than ~5 m) depths (especially see Caysloft Reef area, top right inset in Fig. 4), where the modified $K_d$ Lee(488) may even show larger errors than the standard $K_d$ Lee(488). Further, these maps must be viewed with caution — although they show $K_d(488)$ derived for all pixels in the scene, the algorithm has only been validated for bottoms deeper than 5 m. Focusing only on such waters (~5-30 m depth), percent difference calculations show that the standard $K_d$ Lee algorithm overestimates the true $K_d(488)$ by a factor of 2 throughout much
Table 2
Summary of statistics for concurrent satellite and in situ measurements of multiplex K_d

<table>
<thead>
<tr>
<th>Band</th>
<th>Range</th>
<th>N</th>
<th>R^2</th>
<th>Slope</th>
<th>Intercept</th>
<th>p-Value</th>
<th>Mean ratio</th>
<th>STDY ratio</th>
<th>URMS (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard K_d, Lee (common)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K_d(412)</td>
<td>0.07-0.46</td>
<td>31</td>
<td>0.06</td>
<td>0.28</td>
<td>0.25</td>
<td>0.44</td>
<td>1.68</td>
<td>0.04</td>
<td>0.62</td>
</tr>
<tr>
<td>K_d(412)</td>
<td>0.05-0.24</td>
<td>32</td>
<td>0.13</td>
<td>0.22</td>
<td>0.12</td>
<td>0.05</td>
<td>1.67</td>
<td>0.07</td>
<td>0.55</td>
</tr>
<tr>
<td>K_d(488)</td>
<td>0.05-0.20</td>
<td>32</td>
<td>0.19</td>
<td>0.16</td>
<td>0.08</td>
<td>0.03</td>
<td>0.60</td>
<td>0.08</td>
<td>0.50</td>
</tr>
<tr>
<td>K_d(531)</td>
<td>0.07-0.17</td>
<td>32</td>
<td>0.47</td>
<td>0.08</td>
<td>0.06</td>
<td>0.04</td>
<td>1.32</td>
<td>0.33</td>
<td>0.32</td>
</tr>
<tr>
<td>K_d(547)</td>
<td>0.08-0.16</td>
<td>32</td>
<td>0.41</td>
<td>0.64</td>
<td>0.06</td>
<td>0.03</td>
<td>1.52</td>
<td>0.38</td>
<td>0.28</td>
</tr>
<tr>
<td>K_d(555)</td>
<td>0.07-0.16</td>
<td>32</td>
<td>0.47</td>
<td>0.61</td>
<td>0.07</td>
<td>0.03</td>
<td>1.72</td>
<td>0.23</td>
<td>0.28</td>
</tr>
<tr>
<td>K_d(645)</td>
<td>0.34-0.42</td>
<td>5</td>
<td>0.09</td>
<td>2.76</td>
<td>-0.39</td>
<td>0.62</td>
<td>1.79</td>
<td>0.75</td>
<td>0.58</td>
</tr>
<tr>
<td>K_d(670)</td>
<td>0.42-0.53</td>
<td>7</td>
<td>0.18</td>
<td>3.35</td>
<td>-1.00</td>
<td>0.34</td>
<td>1.70</td>
<td>0.68</td>
<td>0.56</td>
</tr>
<tr>
<td>K_d(670)</td>
<td>0.46-0.53</td>
<td>9</td>
<td>0.02</td>
<td>-3.27</td>
<td>2.80</td>
<td>0.73</td>
<td>2.20</td>
<td>1.36</td>
<td>0.74</td>
</tr>
<tr>
<td>Modified K_d, Lee (common)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K_d(412)</td>
<td>0.07-0.46</td>
<td>31</td>
<td>0.92</td>
<td>0.04</td>
<td>&lt;0.01</td>
<td>1.00</td>
<td>0.03</td>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td>K_d(443)</td>
<td>0.06-0.34</td>
<td>35</td>
<td>0.74</td>
<td>0.06</td>
<td>&lt;0.01</td>
<td>0.89</td>
<td>0.25</td>
<td>0.31</td>
<td></td>
</tr>
<tr>
<td>K_d(469)</td>
<td>0.05-0.25</td>
<td>32</td>
<td>0.65</td>
<td>1.10</td>
<td>-0.61</td>
<td>0.07</td>
<td>0.97</td>
<td>0.28</td>
<td></td>
</tr>
<tr>
<td>K_d(488)</td>
<td>0.05-0.20</td>
<td>32</td>
<td>0.70</td>
<td>0.06</td>
<td>0.00</td>
<td>&lt;0.01</td>
<td>0.58</td>
<td>0.37</td>
<td>0.26</td>
</tr>
<tr>
<td>K_d(531)</td>
<td>0.07-0.16</td>
<td>32</td>
<td>0.52</td>
<td>1.15</td>
<td>-0.63</td>
<td>0.01</td>
<td>0.79</td>
<td>0.34</td>
<td>0.49</td>
</tr>
<tr>
<td>K_d(547)</td>
<td>0.07-0.16</td>
<td>32</td>
<td>0.34</td>
<td>0.97</td>
<td>-0.62</td>
<td>0.06</td>
<td>0.79</td>
<td>0.36</td>
<td>0.53</td>
</tr>
<tr>
<td>K_d(555)</td>
<td>0.07-0.16</td>
<td>32</td>
<td>0.29</td>
<td>0.69</td>
<td>-0.61</td>
<td>0.09</td>
<td>0.83</td>
<td>0.41</td>
<td>0.55</td>
</tr>
<tr>
<td>K_d(645)</td>
<td>0.34-0.42</td>
<td>5</td>
<td>0.09</td>
<td>-0.38</td>
<td>0.61</td>
<td>0.63</td>
<td>1.16</td>
<td>0.17</td>
<td>0.19</td>
</tr>
<tr>
<td>K_d(667)</td>
<td>0.42-0.51</td>
<td>7</td>
<td>0.23</td>
<td>0.34</td>
<td>0.39</td>
<td>0.28</td>
<td>1.14</td>
<td>0.08</td>
<td>0.15</td>
</tr>
<tr>
<td>K_d(670)</td>
<td>0.46-0.53</td>
<td>9</td>
<td>0.07</td>
<td>-0.20</td>
<td>0.43</td>
<td>0.51</td>
<td>1.13</td>
<td>0.07</td>
<td>0.14</td>
</tr>
<tr>
<td>Modified K_d, Lee (all)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K_d(412)</td>
<td>0.05-0.46</td>
<td>24</td>
<td>0.78</td>
<td>0.70</td>
<td>0.01</td>
<td>&lt;0.01</td>
<td>0.64</td>
<td>0.24</td>
<td>0.36</td>
</tr>
<tr>
<td>K_d(443)</td>
<td>0.05-0.34</td>
<td>28</td>
<td>0.70</td>
<td>0.79</td>
<td>0.01</td>
<td>&lt;0.01</td>
<td>0.86</td>
<td>0.24</td>
<td>0.34</td>
</tr>
<tr>
<td>K_d(469)</td>
<td>0.05-0.25</td>
<td>22</td>
<td>0.75</td>
<td>0.90</td>
<td>0.00</td>
<td>&lt;0.01</td>
<td>0.93</td>
<td>0.26</td>
<td>0.28</td>
</tr>
<tr>
<td>K_d(488)</td>
<td>0.05-0.20</td>
<td>22</td>
<td>0.68</td>
<td>0.95</td>
<td>0.00</td>
<td>&lt;0.01</td>
<td>0.93</td>
<td>0.37</td>
<td>0.51</td>
</tr>
<tr>
<td>K_d(531)</td>
<td>0.05-0.16</td>
<td>20</td>
<td>0.40</td>
<td>0.90</td>
<td>-0.61</td>
<td>&lt;0.01</td>
<td>0.83</td>
<td>0.31</td>
<td>0.44</td>
</tr>
<tr>
<td>K_d(547)</td>
<td>0.05-0.16</td>
<td>20</td>
<td>0.18</td>
<td>0.40</td>
<td>0.02</td>
<td>-0.06</td>
<td>0.06</td>
<td>0.78</td>
<td>0.33</td>
</tr>
<tr>
<td>K_d(555)</td>
<td>0.05-0.16</td>
<td>18</td>
<td>0.21</td>
<td>0.83</td>
<td>0.01</td>
<td>&lt;0.01</td>
<td>0.88</td>
<td>0.34</td>
<td>0.45</td>
</tr>
<tr>
<td>K_d(645)</td>
<td>0.34-0.45</td>
<td>6</td>
<td>0.19</td>
<td>0.53</td>
<td>0.66</td>
<td>0.39</td>
<td>1.13</td>
<td>0.28</td>
<td>0.18</td>
</tr>
<tr>
<td>K_d(667)</td>
<td>0.42-0.55</td>
<td>13</td>
<td>0.02</td>
<td>0.10</td>
<td>0.59</td>
<td>0.66</td>
<td>1.14</td>
<td>0.11</td>
<td>0.16</td>
</tr>
<tr>
<td>K_d(670)</td>
<td>0.36-0.57</td>
<td>13</td>
<td>0.30</td>
<td>0.74</td>
<td>0.19</td>
<td>0.05</td>
<td>1.12</td>
<td>0.07</td>
<td>0.13</td>
</tr>
</tbody>
</table>

Range shows spread of in situ measurements; N = number of matchups; R^2 = coefficient of determination; URMS = unexplained two mean squared percent difference (see Section 3.4 for details). *versus* indicates in situ measurements with quality controlled satellite K_d from both algorithms.

of the FRT, and especially in spring and summer (Fig. 5 right column). This is especially true for the Upper Keys and Biscayne Bay regions, where three- to four-fold errors in standard K_d, Lee retrievals are common.

Application of the modified K_d, Lee algorithm, however, does affect K_d retrievals for waters outside the FRT (Fig. 5). In the percent difference images, this is especially prevalent for the West Florida Shelf (WFS) and north of the Lower Keys islands during spring and summer months, but also can be seen in the extremely clear and deep waters of the Florida Straits (Fig. 5 right column). The difference in K_d retrievals from the two algorithms for these regions is typically less than ±50% (compared to 100–400% within the FRT). As the water is extremely clear when and where these differences outside the FRT occur, the discrepancy in K_d between the two satellite algorithms in these instances is typically <0.02 m^−1. For comparison, within the FRT region, this difference typically ranges from 0.06 to 0.12 m^−1. Many coastal regions of mainland Florida, including Biscayne and...
Florida Bays, also show large (up to 0.1 m\(^{-1}\)) differences between the two algorithms, which are not seen in the percent difference images due to the overall high \(K_d(488)\) values in these regions.

The modified algorithm did not improve \(K_d\) retrievals equally for all wavelengths. The most prominent improvements were seen in the shorter (<500 nm) wavelengths, but results were mixed for other wavelengths. For longer wavelengths (>600 nm), there was little difference between the \(R^2\) and linear regression statistics for the standard and modified algorithms. However, coupling the other statistical indices (mean ratio, standard deviation ratio, and RMS) with the graphical representation of matchups shows that the modified algorithm calculates \(K_d\) closer to the in situ values than does the standard \(K_d\) [Lee]. Nevertheless, the modified \(K_d\) [Lee] cannot resolve the variation in these data points because within such clear waters, \(K_d\) in these longer wavelengths is dominated by the constant water absorption coefficient. Lastly, neither the standard nor modified \(K_d\) [Lee] showed marked improvement over the other in the green wavelengths (531, 547, and 555 nm). This is partially due to the exclusion of MODIS/A data for spatial heterogeneity, which occurred more frequently for the standard than the modified \(K_d\) [Lee]. Indeed, restricting the statistical analyses to the matchups used in the standard algorithm validation yields greatly improved performance from the modified method.

The sensitivity simulation was used to investigate the relative performance of the two algorithms without in situ measurement error or differences in numbers of validation points. The results from this simulation (Fig. 6) indicate that the modified \(K_d\) [Lee] tends to slightly underestimate the true \(K_d\) in most normal FRT water, while the opposite is seen for the standard \(K_d\) [Lee]. In the blue and green wavelengths and deeper waters (>10 m), the magnitude of the error is approximately equal for these two algorithms. Shallower depths (<10 m), however, show much larger errors in the standard \(K_d\) [Lee] at all wavelengths; clearly a result from bottom reflectance [perceived as higher \(b_{so}\) and \(a_d\) throughout the standard QA4 algorithm]. The underestimation by the modified \(K_d\) [Lee], on the other hand, was an expected result of bottom contribution in the shorter wavelengths. This is due to the fact that even if water properties at the reference wavelength are stable, measured \(R_{so}\) in the shorter wavelengths has been impacted by benthic contributions. As a result, although \(a_d/\text{ref}\) and \(b_{so}/\text{ref}\) are reasonably estimated, lower \(a_d/\lambda\) (Eq. 7) would be resulted from an elevated \(u(\lambda)/\text{ref}\) (Eq. 5) where the \(K_d\) have extra contributions from the benthos. Lower \(a_d/\lambda\) will subsequently result in an underestimation of \(K_d\) for shorter wavelengths (Eq. 1). Despite this underestimation, the bias of the modified \(K_d\) [Lee] is relatively stable with increasing benthic albedo compared to the standard \(K_d\) [Lee], especially at shallower depths. It is important to note that although a range of benthic albedo values from 0 to 50% is shown in Fig. 6, the spatial heterogeneity of benthic environments in the FRT (and other coral reef systems) means that it is unlikely that either of these extremes in benthic albedo would be reached for a 250 m x 250 m pixel. Finally, simulated standard \(K_d\) [Lee] in the red wavelengths showed extremely large errors with increasing benthic albedo, while the modified \(K_d\) [Lee] showed almost no errors. Overall, this simulation highlighted the failures of the standard \(K_d\) [Lee] in response to bottom contamination, while demonstrating improved performance of the modified \(K_d\) [Lee], especially in very shallow waters and in the red wavelengths.

3.8 Application considerations

The modified algorithm described here can be used to derive the diffuse attenuation coefficient in clear shallow waters (>5 m depth), and shows substantial improvement over the standard \(K_d\) [Lee] in several wavelengths. Implementation of this algorithm requires \(R_{so}\) data at
only three bands (centered at 443, 547, and 667 nm for MODIS), which can then be applied to any other visible band (e.g., 488). These, or similar, bands are within the ongoing data streams from the MODIS instruments on both Aqua and Terra, as well as in the historical Coastal Zone Color Scanner (CZCS), Sea-Viewing Wide Field of View Sensor (SeaWiFS, 1997–2010), and Medium Resolution Imaging Spectrometer (MERIS, 2002–2012) datasets. Further, this algorithm lends itself to application using data from the Visible Infrared Imaging Radiometer Suite (VIIRS, 2011–present) instrument for ongoing and future assessment of water clarity in optically shallow environments. Finally, as in situ measurements of \( K_\text{d} \) in optically shallow waters may have large errors due to wave-focusing throughout the water column, this technique may also be applied to shipborne \( K_\text{d} \) measurements. Concurrent with \( E_z \) profiles, such application would provide independent verification of the \( E_z \)-derived \( K_\text{d} \).

The validation dataset was collected in optically shallow waters south and east of the Florida Keys (5–30 m depth), and showed large differences in \( K_\text{d}(488) \) retrievals between the standard and modified algorithms. Outside this FRT region, with some exceptions (notably, WFS in spring and nearshore mainland Florida), there is widespread agreement between the standard and modified \( K_\text{d} \). Since the standard \( K_\text{d} \) algorithm has been validated in this region (Zhao et al., 2013), such agreement indicates increased applicability of the modified algorithm, both outside the FRT (spatially) and beyond the range of its validation dataset. Similarly, due to the local validation of the standard \( K_\text{d} \), exceptions to this agreement indicate bounds for the potential applicability of the modified algorithm. Specifically, \( K_\text{d} \) retrievals from the modified algorithm for extremely shallow and highly attenuating waters (Biscayne and Florida Bays, as well as nearshore mainland Florida) are likely erroneously overestimated. For other regions of disagreement, such as the WFS in spring, we find that the scale of the difference is not sufficient to justify a switch to the standard \( K_\text{d} \).

Although not directly tested against in situ data from other regions, we feel that the modified \( K_\text{d} \) would yield similar improvements in water clarity retrievals for other optically shallow environments. To illustrate this potential applicability, a MODIS/Aqua pass including the Belize Barrier Reef region was processed using the standard and modified \( K_\text{d} \) (Fig. 7). Although no bathymetric data were available for this region, pixels which showed high \( K_\text{d}(488) \) derived using the standard \( K_\text{d} \) appear to co-occur with areas where the bottom is clearly visible in the true color image. Using the modified algorithm, many of these apparently artificially elevated \( K_\text{d} \) measurements do not appear to be influenced by bottom contamination. However, as seen in the FRT (Gatafort reef areas, Figs. 4 & 5), even larger errors in \( K_\text{d} \) products are seen for extremely shallow regions using the modified algorithm. Nevertheless, given the extremely large bottom reflectance signal compared to water column reflectance for shallow (>5 m) clear waters, accurate water property retrievals at these locations from ocean color data still requires further research, for example by explicitly taking into account both bottom depth and albedo in the algorithm development.

4. Spatiotemporal water clarity patterns in the Florida Keys

4.1. Analysis methods

A number of techniques were utilized to investigate the spatial and temporal variability of \( K_\text{d} \) (derived using the modified \( K_\text{d} \)) in the Florida Keys region. Variation in \( K_\text{d} \) at 488 nm is used in this analysis
because historically $K_{d}(490)$ or $K_{d}(488)$ has been used as a measure of water clarity. Light at 488 nm is within the transparency window for most waters, allowing light to reach the benthos in the FRT region.

To visualize temporal water clarity variations in this region, the monthly summaries of $K_{d}$ statistics were investigated along an approximate 10 m bathymetric isobath, derived from a raster bathymetry created by Palandro (2006). For each pixel along this transect, monthly mean $K_{d}$ from each month of MODIS/A data (July 2002 to Dec 2011) were extracted. This same data extraction was implemented for $K_{d}$ monthly anomaly, standard deviation, and coefficient of variation data.

An empirical orthogonal function (EOF) analysis was used to explore spatiotemporal groupings in water clarity. The singular value decomposition method was used for computational efficiency (Kelly, 1988). Using ENVI (version 4.8; Exelis Visual Information Solutions) and the raster bathymetry, a region of interest (ROI) was created which included only waters south and east of the Florida Keys/Dry Tortugas and with depths of 5 to 30 m, roughly corresponding to the FRT extent. Monthly chlorophyll data within this ROI were sorted into ASCII text files along with their latitude and longitude. As the EOF analysis requires no gaps in data coverage, any pixel with monthly chlorophyll data for every month was excluded. The EOF was then performed on this gridded time series, resulting in twelve principal component axes (modes). Using the retained latitude and longitude, the pixel distances along each mode was color coded, re-engaged to the original position and saved as PNG files. Also recorded was the percentage of total variation described by each mode (eigenvalue), as well as the time series of monthly relative amplitudes of the data within the mode.

Finally, a two-way ANOVA was performed using Mathlab® (version 2013a) to evaluate regional variation in water clarity across the FRT regions (see Fig. 10). The independent variables for this test were groupings by region (Biscayne Bay, Upper, Middle and Lower Keys, Marquesas, and Dry Tortugas) and by linear distance to the closest land pixel. Linear distance from land was binned into groups 0–4 km, 4–8 km, 8–12 km, and only waters with bottom depths of 5–30 m were considered. The dependent variable was the average of all (2002–2011) $K_{d}(488)$ data at each pixel. Eilllerers and Kruskal–Wallis tests were performed to assess data conformance to ANOVA assumptions of normality and homoscedasticity, respectively. Although many groups showed failure to meet one or both of these assumptions, the large number of data points and robustness of the ANOVA in such situations (Sokal & Rohlf, 1981) allowed for its appropriate implementation. The null hypothesis of this test was equal water clarity across regions and with distance from shore. Tukey’s pairwise comparisons were performed to elucidate significant differences between individual groups.

4.2. Spatiotemporal patterns

The time series of climatology images (Fig. 5) show that clear water persists throughout the year for most of the region, with $K_{d}(488)$ generally less than 0.5 m$^{-1}$. The main gradient in water clarity is from high inshore to low offshore. Spring and summer months have the clearest waters, while winter months have the highest $K_{d}(488)$ regionally.

Along the 10 m transect, mean monthly data (Fig. 8d) again show extremely clear waters in the Upper and Middle Keys, as well as some of the same seasonal variation described above. The Upper Keys region has the clearest waters, with water clarity decreasing and becoming more variable (Fig. 8d) westward along the transect. Coefficient of variation (Fig. 8e) shows consistent scale and variability throughout time along this transect, indicating that $K_{d}(488)$ variability is strongly correlated to the mean $K_{d}(488)$.

The EOF analysis was performed so that variation within this complex system could be summarized. Mode one of the EOF explained over 85% of the variation, and its eigenvector amplitudes by month indicated that this represents a smooth seasonal cycle. EOF mode two explained 9% of the total variance, and all other modes explain less than 1%. With this quantity of data (over 60,000 pixels during each of 12 months), 100 EOF analyses performed on randomly generated noise indicated that with 95% confidence, modes with eigenvalues explaining 9% or less of the variation are non-significant. Thus all modes except mode one (the seasonal cycle) were considered non-significant. As a result, a simple harmonic equation was fit to the data to describe the seasonal cycle elucidated by EOF mode one. At each pixel, the sum of squares was minimized to best fit a simple harmonic oscillation:

$$x = X + A \cos(2\pi t + \phi) + B \sin(2\pi t + \phi),$$

where $x$ is the satellite-derived climatology mean $K_{d}(488)$ from a particular month and pixel, $X$ is the average of monthly climatologies at that pixel, $t$ is time in months, and $A$ and $B$ are the pixel-specific amplitude and phase of the oscillation calculated and mapped (Fig. 9). In this visualization, amplitude represents one-half of the range of best-fit $K_{d}(488)$ values, and phase shows the timing (in months) of the maximum of this harmonic.

Finally, the two-way ANOVA showed significant effects of both region ($F = 3651$; $p = 0.0001$) and distance from shore ($F = 10280$; $p = 0.0001$) but also indicated a significant interaction ($F = 458$; $p = 0.0001$) between these two factors. As such, individual one-way ANOVAs were performed on data from each of the factor group levels. Within each region, there was a strongly significant effect of distance from land (ANOVA for each region showed $F > 700$ with 2 d.f. and
p < 0.0001), and a common trend of decreasing $K_d$ with distance from land. Pairwise comparisons on each regional analysis showed that each grouping by distance from land was significantly different (i.e., the 0–4 km pixels within a region always had significantly higher $K_d$ than the 4–8 km pixels, both of which were significantly higher than the 8–12 km pixels). Holding the distance from land group constant, ANOVAs performed on individual regions also showed strongly significant effects ($df = 5$; $F > 800$; $p < 0.0001$ for each ANOVA; Fig. 10). For the nearshore (0–4 km) pixels, pairwise comparisons indicated that each region was significantly different from all others, with the Dry Tortugas showing the lowest $K_d$ and Marquesas having the highest. Excluding the Dry Tortugas region, $K_d$ significantly decreased for every region in a sequential manner northeast along the FRT (Fig. 10). This general pattern was seen for both the 4–8 km and 8–12 km groups, with some exceptions (most notably, no statistically significant difference between Middle Keys and Biscayne Bay waters 4–8 km from land).

4.3. Discussion

Together, these analyses and visualizations present a picture of clear water region-wide with generally low spatiotemporal variability. Nevertheless, validated synoptic $K_d$ data can be used to detect significant differences between regions. Because data were grouped according to their traditionally defined regions (Klein & Orlando, 1994) for the ANOVA analyses, direct comparison to previous works was possible. As such, we find that the widely held hypotheses of poorest water clarity in the Middle Keys region (see Lapointe & Clark, 1992) and clearest water in the Lower Keys (see Boyer & Jones, 2002; Klein & Orlando, 1994; Szman & Forrester, 1996) need revision. This analysis, however, does find increasing water clarity (decreasing $K_d$) with distance from shore, in agreement with previous studies (Lapointe & Clark, 1992; Szman & Forrester, 1996). Also, this analysis of $K_d$ concurs with the conclusion of Boyer and Jones (2002) that the Marquesas region has the highest chlorophyll concentrations.

Even though some of the relative regional differences in water clarity identified in the current work differ from the results of previous analyses of water clarity (Boyer & Jones, 2002; Klein & Orlando, 1994; Lapointe & Clark, 1992; Szman & Forrester, 1996), the noted spatiotemporal trends are in accordance with regional circulation patterns (see Lee, 2013; Lee & Smith, 2002; Lee & Williams, 1999; Lee, T., et al., 2002; Porter et al., 1999; Smith, 1994). Specifically, although there is a net flow of water southward through the channels separating the Florida Keys islands, the strongest of such transports are in the
Fig. 9. EOF analysis showed singular importance of a regular seasonal cycle. Maps depict the: a) amplitude and (inter: map, b) phase of a single harmonic oscillation fit to describe this cycle in $K_{4}(488)$ for waters with depth between 5 and 30 m. Phase is shown as month of maximum $K_{4}(488)$. Land shown in black with a white coastline. No data shown as gray.

winter and spring (Lee, T., et al. 2002). Also, the shifting of average winds from southeasterly in the summer to easterly or northeasterly in the winter brings a reversal in flow in the Middle Keys from northward to southward (Lee, 2012). As such, in winter when the largest influxes of water are flowing into the FRT region through the Middle Keys channels, strong alongshore currents are moving this water towards the Lower Keys and Marquesas Keys regions, which can potentially explain the maxima in $K_{4}(488)$ noted in the Lower Keys during winter.

More importantly, however, the large quantity of data provided by MODIS/A and this modified $K_{4}$ Lee algorithm allows for more robust zonation than the traditional region designations. Within any region, sub-regions can be pinpointed which show large differences in climatology and seasonal cycle amplitude. For example, harmonic analyses showed distinct groups according to their seasonal variation, with offshore areas having the most stable water clarity (low amplitude) and inshore waters being more variable. As was seen in the mean climatologies, this is especially true in the Middle and Lower Keys, nearest the main thoroughfares for water leaving Florida Bay. The Upper Keys region appears to lack those high amplitudes in nearshore regions, which may result from a lack of large channels for water influx. Alternatively, the masking of pixels less than 5 m depth in these analyses may partially be obscuring nearshore amplitude highs in the Upper Keys. Nevertheless, the data volume provided by this method allows for testing of statistical differences between individual reef or seagrass environments, and retrospective analysis of their light exposure history.

Temporally, the EOF analysis indicated that a smooth seasonal cycle is the prevailing mechanism explaining water clarity variations. The phase of this variation shows nearly ubiquitous $K_{4}(488)$ maxima in the winter. November, December, and January were the peak $K_{4}(488)$ months for 8, 69, and 14% of pixels, respectively (all other months...
were less than 1.5%). The Middle and Lower Keys region seems to peak earlier (November or December) than the waters to the north and to the west. Further, the time-space visualizations (Fig. 8) allow for assessment of anomalous water clarity events. The most prominent features in water clarity along the 10 m isobath are a sharp increase in mean and standard deviation of \( K_s' \) (488) west of approximately 87.75° W latitude (near Key West), as well as a series of low water clarity events (Fig. 8c). The former is potentially due to influxes of water from Key West and Boca Grande Channels, and agrees with other analyses showing low water clarity in the Lower Keys and Marquesas regions (Boyer & Jones, 2002). This effect could potentially be amplified by proximity to land. The 10 m transect is closer to land in the Lower Keys than in the Upper Keys, which could have the effect of capturing waters affected by land-based nutrient sources, especially the population center of Key West. Again, the ANOVA analysis showed that, regardless of region, proximity to land has a significant effect on water clarity.

The large anomalies in water clarity seen in late 2003, late 2005, and early 2010 along the 10 m isobath can be traced to particular events. First, in late 2003 a dark plume of water was observed to flow from the SW Florida coast into the Dry Tortugas region by late October (Hu et al., 2004) explaining the anomaly in derived water clarity at that time frame. The largest anomaly in water quality was seen in late 2005, due to Hurricane Wilma that passed just north of the Florida Keys in mid-October. This hurricane caused a rise in water level within Florida Bay, which overwashed most of the Middle and Lower Keys, likely leading to an extremely turbid and nutrient-rich environment. Finally, February and March of 2010 show high anomalies due to an extremely large and previously unreported, influx of low clarity water through the channels in the Middle Keys. This plume is clearly visible in true color satellite imagery. It is possible that the extreme cold event in January 2010 (see Barnes & Hu, in press; Barnes et al., 2011; Lirman et al., 2011) caused mortality of Euphyllia flabellata and subsequent nutrient release (Queumer et al., 1994). If advected into the FRT region, colored dissolved organic material (CDOM) from the plant decay or phytoplankton blooms stimulated by the influx of nutrients could cause the anomalously high \( K_s' \) (488) observed.

4.4. Implications

Despite the wealth of scientific research describing the interactions between light and coral reef health, many such investigations are based on an individual coral colony (e.g., Lesser et al., 1990), samplings of adult tissue (e.g., Hoehl-Gudberg & Jones, 1999) or larvae microcosms (e.g., Gleason et al., 2006). Unfortunately, more robust analyses are impossible because current water clarity datasets are insufficient to quantitatively assess long-term and region-wide light availability. Further, current datasets are mostly derived from long-term monitoring programs or from submerged sensor arrays, both of which are expensive and labor intensive. The algorithm described in this work adds an unprecedented amount of historical and ongoing information about the water clarity in coral reef environments, with minimal additional cost. Combined with bottom depth and satellite-derived \( K_s \), the multispectral light environment surrounding corals can be estimated from CAXS, SeaWiFS, MODIS, MERIS, and VIRS data using this modified algorithm, although performance may be limited by the signal-to-noise ratio of the particular instrument. As a result, the relative paucity of in situ light attenuation data may no longer be a factor hindering our understanding of region-wide effects of light on corals at > 5 m water depth, at least for the Florida Keys.

To date, large scale investigations of declines in coral reef health have focused almost singularly on sea surface temperature (SST; e.g., Liu et al., 2005). This is driven partially by the large impact of temperature on coral health, but also by the widespread availability of validated satellite SST data (as opposed to \( K_s' \) data). The modified water clarity algorithm allows for robust understanding of the individual and combined effects of specific light and temperature events on corals, as well as the impacts of long-term exposures. Such information could be used to create a metric for coral health which could be assessed using satellite data in near real-time.

Beyond scientific applications for the algorithm itself, the spatiotemporal patterns of water clarity in the FRT region are significant in that they depart from current conceptions about the region. The new paradigm offered in this paper describes a mainly onshore-offshore gradient in water clarity throughout the region, but also transitions in both water clarity and variability along the reef tract. As generally understood, the large discharge channels from Florida Bay greatly affect FRT waters, and indeed are driving the separation between these regions or sub-regions. Their impact is spread throughout much of the Middle and Lower Keys region, as well as the Marquesas region.

Applied to current monitoring efforts and to the ongoing re-sensing process for the FRMMS, these new satellite-based water clarity results can have significant impacts. The overall goal of these programs is to preserve native resources. Even in the absence of detailed information about the region wide impacts of current and long-term exposure to specific light regimes, the regional differences in FRT water clarity can inform these preservation efforts. Specific zones for preservation or restoration should include reefs within extremely clear waters, where corals have traditionally thrived, but also reefs acculturated to water clarity regimes which are more variable and highly attenuating (particularly nearshore). In the FRMMS, reefs in such environments currently exhibit significantly higher coral cover and coral growth rates than those in traditional offshore environments (Lirman & Feng, 2007), and as such may show resilience to potential future water clarity variability.

5. Conclusion

We have tested a modified algorithm which shows improvement in satellite derived \( K_s \) in optically shallow waters for several wavelengths, allowing widespread current and historical assessment of the light environment experienced by benthic ecosystems. This new product can further be used to investigate spatiotemporal patterns in water clarity. Within the FRT region in the Florida Keys, such analysis challenges some published accounts describing the relative clarity of the traditional geographic regions, which can have large and immediate impacts on the management of shallow marine systems. Research and monitoring efforts will benefit from combining satellite-based temperature data with this new water clarity data to allow widespread assessment of coral reef and seagrass environments in near-real time.

Acknowledgments

This work was supported by the U.S. National Aeronautics and Space Administration through its Decision Support program, Gulf of Mexico program, Ocean Biology and Biogeochemistry program, and Water and Energy Cycle program. The authors wish to thank Caityun Zeng (Tsinghua University, China) for providing the EOF routines and Gary Milliman (University of South Florida) for assistance in EOF and harmonic oscillation analyses, as well as the anonymous reviewers whose comments helped to greatly improve this work. Coastline shape files were acquired from the NOAA National Geophysical Data Center (Wessell & Smith, 1996) and the Florida Fish and Wildlife Conservation Commission.

References


APPENDIX D:

ESTIMATION OF THE DIFFUSE ATTENUATION COEFFICIENT OF ULTRAVIOLET LIGHT IN
OPTICALLY SHALLOW FLORIDA KEYS WATERS FROM MODIS MEASUREMENTS

Estimation of diffuse attenuation of ultraviolet light in optically shallow Florida Keys waters from MODIS measurements

Brian B. Barnes a,*, Chuanmin Hu a, Jennifer P. Cannizzaro b, Susanne E. Craig b, Pamela Hallock a, David L. Jones a, John C. Lehter c, Nelson Melo d, e, Blake A. Schaeffer c, Richard Zepp f

a College of Marine Science, University of South Florida, 1407 7th Avenue South, St. Petersburg, FL 33701, USA
b Dalhousie University, Department of Oceanography, Halifax, Nova Scotia, Canada
c National Health and Environmental Effects Research Laboratory, Gulf Ecology Division, United States Environmental Protection Agency, Gulf Breeze, FL, USA
d Cooperative Institute for Marine and Atmospheric Studies, University of Miami, MIAMI, FL, USA
e National Oceanic and Atmospheric Association Atlantic Oceanographic and Meteorological Laboratory, Miami, FL, USA
f National Exposure Research Laboratory, United States Environmental Protection Agency, Athens, GA, USA

ARTICLE INFO

Article history:
Received 29 May 2013
Received in revised form 13 September 2013
Accepted 25 September 2013
Available online xxx

Keywords:
Water clarity
Light penetration
Ultraviolet light
Remote sensing
Shallow water
Coral reef

ABSTRACT

Diffuse attenuation of solar light ($K_0$, m$^{-1}$) determines the percentage of light penetrating the water column and available for benthic organisms. Therefore, $K_0$ can be used as an index of water quality for coastal ecosystems that are dependent on photosynthesis, such as the coral reef environments of the Florida Reef Tract. Ultraviolet (UV) light reaching corals can lead to reductions in photosynthetic capacity as well as DNA damage. Unfortunately, field measurements of $K_0$(UV) lack sufficient spatial and temporal coverage to derive statistically meaningful patterns, and it has been notoriously difficult to derive $K_0$ in optically shallow waters from remote sensing due to bottom contamination. Here we describe an approach to derive $K_0$(UV) in optically shallow waters of the Florida Keys using variations in the spectral shape of MODIS-derived surface reflectance. The approach used a principal component analysis and stepwise multiple regression to parsimoniously select modes of variance in MODIS-derived reflectance data that best explained variance in concurrent in situ $K_0$(UV) measurements. The resulting models for $K_0$(UV) retrievals in waters 1–30 m deep showed strong positive relationships between derived and measured parameters (e.g., for $K_0$(305)) ranging from 0.28 to 3.27 m$^{-1}$; N = 29; $R^2$ = 0.94]. The predictive capabilities of these models were further tested, also showing acceptable performance (for $K_0$(305), $R^2$ = 0.92; bias = -0.02 m$^{-1}$; $RMS = 0.23$). The same approach worked reasonably well in deriving the absorption coefficient of colored dissolved organic matter (CDOM) in UV wavelengths [$a_\lambda$(UV), m$^{-1}$] as $K_0$(UV) is dominated by $a_\lambda$(UV). Application of the approach to MODIS data showed different spatial and temporal $K_0$(305) patterns than the $K_0$(488) patterns derived from a recently validated semi-analytical approach, suggesting that different mechanisms are controlling $K_0$ in the UV and in the visible. Given the importance of water clarity and light availability to shallow-water flora and fauna, the new $K_0$(UV) and $a_\lambda$(UV) data products provide unprecedented information for assessing and monitoring of coral reef health, and could further assist ongoing regional protection efforts.

© 2013 Elsevier Inc. All rights reserved.

1. Introduction

The necessity of light for photosynthetic energy creation restricts zooxanthellate corals to shallow, oligotrophic environments which can present potential exposure to ultraviolet (UV) radiation. While light is critical for photosynthesis, exposure to intense UV radiation can cause oxidative stress (Feyer, Lelandais, & Kunert, 1994; Jokiel, 1980) in corals and other reef flora (Fisk & Done, 1985; Hoegh-Guldberg & Jones, 1999; Lesser, Stoich, Tapley, & Shick, 1990). Tolerance to incident UV radiation may depend on the concentration of colored dissolved organic matter (CDOM, aka gelbstoff or yellow matter) within the surrounding water column (West & Salm, 2003; Zepp et al., 2008). CDOM is a byproduct of terrestrial or marine plant matter decay (Shank, Lee, Vallat, Zemp, & Barrett, 2010). Spectrally, the CDOM absorption coefficient ($a_\lambda$) is the highest in the UV wavelengths, and it decreases with increasing wavelength with an exponential spectral slope (S. Brincaud, Morel, & Prieur, 1981). Exposure to UV light, especially in stratified surface waters, will cause photobleaching and oxidation of CDOM (Fichot & Benner, 2012; Häder et al., 1988; Morán & Zepp, 1997; Shank, Zemp, Vallat, Lee, & Baret, 2010; Zepp et al., 2008), which will subsequently reduce the CDOM-induced light attenuation and increase the UV light potentially reaching coral reef environments.

Despite the wealth of scientific literature describing the relationship between light and coral health, there are surprisingly few implemented
programs to monitor light availability at coral reefs, primarily due to logistical and financial constraints. To overcome this difficulty, the U.S. NOAA’s Coral Watch Program has implemented an experimental light stress product over the global ocean (http://coralreefwatch.noaa.gov/satellite/bd/index.html). However, the product is only based on satellite-estimated surface photosynthetically available radiation in the visible wavelengths (PAR) without accounting for spatial variation in light attenuation or for depth-dependent changes in radiation reaching the benthos, noted by Ventsch et al. (2002) as crucial for all coral studies. This omission is due to a lack of reliable algorithms to derive light attenuation (or water clarity) from satellite data in optically shallow environments (see Barnes et al., 2013; Zhao, Barnes, et al., 2013). Optically shallow is defined here as waters where the bottom is visible from an above-water instrument, which includes the environments inhabited by many zoanthellate corals. This lack of satellite water clarity data stands in direct contrast to sea surface temperature (SST) data from satellites, which are not adversely affected in optically shallow environments (e.g., Hu et al., 2000). As a result, data products based on satellite-derived SST are currently used almost exclusively to predict coral bleaching (see Strong, Liu, Meyer, Hendler, & Sasin, 2004; Strong, Liu, Skirving, & Eakin, 2011).

Estimation of water clarity or diffuse light attenuation coefficient ($K_d$ m$^{-1}$, see Table 1 for list of symbol definitions) in optically shallow environments from satellite measurements has been problematic in the past due to bottom contamination of the satellite-derived remote sensing reflectance ($R_b$). Most inversion algorithms are developed and validated for waters without the benthic contribution to $R_b$. For example, Johannessen et al. (2003) described an empirical relationship between $K_d$(UV) and a reflectance ratio between the blue and green wavelengths for optically deep waters ranging from turbid estuaries to offshore oligotrophic. However, benthic albedo varies with wavelength for disparate bottom types (see Hodson, Arkason, & Andreou, 2003; Werdell & Roesler, 2001). As a consequence, application of the Johannessen et al. (2003) algorithm to optically shallow waters is likely to produce large errors in the retrieved $K_d$(UV). Fig. 1 shows performance of this algorithm in optically shallow waters, using data collected for this study. Benthic contamination has similarly been shown to cause errors in retrievals of water-column chlorophyll-a concentrations (Cannizzaro & Carder, 2006; Cannizzaro et al., in press; Carder, Cannizzaro, & Lee, 2005; Hu, 2008; Schaeffer, Hagy, Connor, Lebret, & Stumpf, 2012) and $K_d$ in visible wavelengths (Zhao, Barnes, et al., 2013). Similar errors are likely to occur for $K_d$(UV) retrievals using other empirical algorithms (e.g., Fichot, Sathyendranath, & Miller, 2008; Smyth, 2011) because of the bottom interference.

Nevertheless, instruments such as the Moderate Resolution Imaging Spectroradiometer (MODIS) on board the US. National Aeronautics and Space Administration (NASA) satellites Aqua (2002–present) and Terra (2000–present) provide medium-resolution (1 km) $R_b$ data for all of the world’s optically shallow regions once every 1–2 days. In the Florida Keys region, Barnes et al. (2013) described a modified quasi-analytical algorithm (QAA, Lee, Carder, & Armone, 2002) to remove bottom contamination and subsequently derive $K_d$ in the visible from MODIS Aqua (MODIS/A) measurements. However, since MODIS does not collect $R_b$ data in UV wavelengths, estimation of $K_d$(UV) requires an approach which is both resilient to variable bottom contamination and which can extrapolate beyond the measured visible satellite data. While $K_d$(UV) is linearly proportional to $K_d$ in the visible bands ($K_d$(VIS)) in oligotrophic open-ocean waters (Lee et al., 2013), in optically complex environments, spatiotemporal differences between the relative concentrations of various water constituents (see Bricaud et al., 1981; DeGrandpré, Vodacek, Nelson, Bruce, & Blough, 1996) generally preclude use of $K_d$(VIS) to derive $K_d$(UV).

Algorithms based on neural networks (Ioannou, Gileerson, Gross, Moshary & Ahmed, 2011, 2013; Jamet, Lessel, & Dessay, 2012), matrix inversion models (Brandt & Dekker, 2003; Phinn, Dekker, Brandt, & Roelfsema, 2005), or empirical orthogonal functions (EOF; aka principal components analyses), Craig et al., 2012; Fichot et al., 2008; Fischer, Doerffer, & Grassl, 1985; Gower, Lin, & Borstad, 1984; Mueller, 1975; Sathyendranath, Hoge, Platt, & Swift, 1989, 1994; Sathyendranath, Prieur, & Morel, 1989; Toole & Siegel, 2001) have the potential to overcome the difficulty of deriving $K_d$ in optically shallow waters, provided that data from these environments are included in the training datasets. The latter approach, which entails partitioning variations in the measured reflectance through the use of an EOF, has previously been used to estimate water properties in the UV (Fichot et al., 2008). This general approach, including its published variants discussed below, will herein be termed the ‘EOF method.’ The EOF method is used to reduce hyper- or multispectral reflectance data to a few uncorrelated variables (EOF modes, aka eigenvectors), which retain most of the variance in the original data. Assuming that a particular water constituent affects the measured reflectance, varying concentrations of that constituent should be correlated to one or more of the EOF modes.

Although the methodology for application of the EOF method has varied in the past, results have typically shown success of this approach in modeling water parameters. The inputs to the EOF method included measured reflectance ($R$; Gower et al., 1984; Mueller, 1975; Sathyendranath et al., 1994), simulated reflectance (Sathyendranath et al., 1989), simulated radiance ($I$; Fischer et al., 1986), and measured $R_b$ ($R_b$(Craig et al., 2012; Fichot et al., 2008; Toole & Siegel, 2001), from regions ranging from coastal to open ocean. Water parameters derived from the EOF method included secchi disk depth (Mueller, 1976), chlorophyll concentration (Craig et al., 2012), fluorescence (Sathyendranath

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_d$</td>
<td>Diffuse attenuation coefficient for downwelling irradiance</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$E_d$</td>
<td>Downwelling irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$E_d$(UV)</td>
<td>Subsurface downwelling irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$I$</td>
<td>Irradiance</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$R$</td>
<td>Reflectance</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>$R_b$</td>
<td>Remote sensing reflectance</td>
<td>$%$</td>
</tr>
<tr>
<td>$a_t$</td>
<td>Total absorption coefficient</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_g$</td>
<td>Absorption coefficient of gelbstoff (CDOM)</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_{sp}$</td>
<td>Absorption coefficient of suspended particless</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_{pp}$</td>
<td>Absorption coefficient of phytoplankton pigments</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$a_{bc}$</td>
<td>Absorption coefficient of particulate clorophyll</td>
<td>m$^{-1}$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
<td>nm</td>
</tr>
<tr>
<td>$z$</td>
<td>Depth</td>
<td>m</td>
</tr>
</tbody>
</table>
et al., 1989), inherent optical properties (IOPs) including absorption coefficients (Craig et al., 2012) and scattering coefficients (Gower et al., 1984), salinity and nutrient concentrations (Yoder & Siegel, 2001), Kd for both visible and ultraviolet wavebands (Fichot et al., 2008), and others. Fichot et al. (2008) and Craig et al. (2012) further demonstrated the effectiveness of this approach using in situ measured \( \text{Kd} \), which had been resampled to wavelengths of satellite instruments. To our knowledge, however, validation of the EOF method using satellite-derived data as an input (e.g., MODIS \( \text{Kd} \)) has yet to be reported. In the present study, our approach is distinct from other published EOF methods through 1) use of satellite-derived data as input; 2) parsimonious model selection via stepwise forward addition; and 3) measure of the predictive ability of models through leave-one-out cross validation (see Sections 3.3 and 3.4 for details).

Thus, given the pressing need for synoptic information on the UV light field reaching coral reef environments, the objective of this study was to develop and validate an approach to estimate \( \text{Kd} \) and \( \text{a}_\lambda \) in UV wavelengths from MODIS/Aqua measurements over optically shallow waters. The method is based on a new approach to implement the EOF method, as well as extensive field data collected from the Florida Keys region for algorithm tuning and validation.

2. Study area — Florida Keys

At the southern tip of the Florida peninsula are the Florida Keys (Fig. 2), a string of limestone islands at 24 to 26°N and 80 to 83°W. The Florida Reef Tract (FRT) is a series of bank and patch reefs located to the south and east of the Keys and extending west to the Dry Tortugas. The patch reefs are generally nearshore (3–5 km from land), while the larger reef tract is located approximately 8–10 km from the shore (abutting the shelf break) with depths typically ranging from 1 to 30 m. For the purposes of this research, the FRT region is delineated as all waters with depths from 0 to 30 m immediately south and east of the Florida Keys, and extending west to the Dry Tortugas. This designation of 30 m matches the classification of “shallow water” in the satellite ocean color community (see Level-2 processing flag COAST2; Patt et al., 2003). This threshold also is an appropriate delineation for the bounds of optically shallow waters in the FRT, as errors in chlorophyll retrievals due to bottom contamination of satellite \( \text{Kd} \) signals in this region have been found for depths shallower than 25 m (Carentz et al., in press; Scheffer et al., 2012).

3. Methods

3.1. In situ data collection

To include a wide spatial and temporal scope for development of an inversion model applicable to all possible scenarios, in situ data were compiled from a number of different sources. As such, different instruments, data collection protocols, and quality assurance procedures were applied to all in situ data. All data were collected in the southwest Florida region, with an emphasis on the FRT. Overall, 292 different locations (211 in the FRT; see Fig. 2) were visited at least once, and up to 16 times per station, for a total of 540 station visits. Data collected at each station typically included vertical profiles of the downwelling irradiance (\( E_d \)) and water samples for the analyses of IOPs (Table 2). Much of these data, along with the collection and processing methods, have been included in previous publications (Ayoub, 2009; Barnes et al., 2013; Cannizzaro & Carder, 2006; Mueller & Fargion, 2002; Scheffer, Komny, Aukamp, Craven, & Ferer, 2011; Zepp et al., 2008, Zhao, Hu, et al., 2013). As such, the following is a summary of the in situ data collection, where differences in protocol and instrumentation between the data sources are highlighted. For simplicity, wavelength (\( \lambda \)) and depth (\( z \)) notation for IOP and \( E_d \) descriptions are omitted except where necessary.

Between January 2003 and May 2006, \( E_d \) and IOP data with a focus on the UV light environment were collected in the Florida Keys and Dry Tortugas regions by the US Environmental Protection Agency (EPA), the methodology for which has been detailed by Zepp et al. (2008). Briefly, a Satlantic (Halifax, NS, Canada) MicroPro profiler, configured to measure multispectral \( E_d \) primarily in UV wavelengths (at 305, 325, 340, 380, 412, and 443 nm) was deployed for 5-6 casts per station. \( E_d(z) \) measurements were discarded when instrument tilt or roll was greater than 5°. Water samples (approx 5 L) were collected at approximately 1 m depth and subsequently filtered to separate the

---

**Fig. 2.** MODIS/RGB image on 9 January 2009 (18:50 CMT) showing in situ measurement locations within the FRT. Diamonds indicate locations with concurrent satellite/is in situ matchups, with color indicating the presence of the in situ data. White crosses are locations with in situ data but without satellite matchup. Blended charts show histograms of sample location-z (depths and b) bottom types (from Florida Fish and Wildlife Conservation Commission habitat maps). RS = bare substrate, CR = coral reef, PS = patchy seagrass, CS = continuous seagrass, U = unapplicable/interpretation, ND = no data.
Table 2
Description of pilot data.

<table>
<thead>
<tr>
<th>Source</th>
<th>Dates (monthly/year)</th>
<th>Samples</th>
<th>MODIS/A MODIS/A</th>
<th>Instrument</th>
</tr>
</thead>
<tbody>
<tr>
<td>USF</td>
<td>5/4, 7/11, 10/30, 11/11, 12/15</td>
<td>39</td>
<td>4</td>
<td>ND</td>
</tr>
<tr>
<td>NOAA</td>
<td>6/3, 6/13, 7/8, 7/10, 7/11</td>
<td>34</td>
<td>8</td>
<td>Bioluminescent PRR-2000 &amp; PUV-2500:</td>
</tr>
<tr>
<td>AOML</td>
<td>6/1, 7/1, 8/6, 8/11, 9/12</td>
<td>34</td>
<td>8</td>
<td>260-800</td>
</tr>
<tr>
<td>EPA/USF</td>
<td>4/11, 7/12, 8/12</td>
<td>144</td>
<td>34</td>
<td>Atlantic HyperPro</td>
</tr>
</tbody>
</table>

(For data details).

Residual scattering was removed from these spectra by subtracting each wavelength by the mean of each measured value between 790 and 800 nm (Pegau et al., 2003). All E2 profiles were processed to derive Ks via Lambert–Beer’s law (Gordon, 1988; Smith & Baker, 1981), using linear regression between depth and

\[
\ln \left( \frac{E_2(z, \lambda)}{E_2(0, \lambda)} \right)
\]

For the EPA/USF and NOAA/AOML data sources, ln(E2) at several wavelengths for each profile was plotted against measurement depth, and the longest sequence of approximately log-linear decay in E2 was manually selected. Only data within this portion of the profile were used in the derivation of Ks via the linear regression. Also, for the EPA/USF and NOAA/AOML data sources, Ks derived from each station was further assessed for quality control by testing the similarity of replicate profiles (i.e., measurement repeatability). Specifically, \(K_s(\lambda)\) from any station was only considered reliable if the difference in \(K_s(\lambda)\) from two or more replicate profiles was less than 0.01 m^{-1} and/or the coefficient of variation for two or more replicate profiles was less than 10%. The individual \(K_s(\lambda)\) measurements which fit either of these conditions were averaged to yield the final \(K_s(\lambda)\) used in subsequent analyses. In the NOAA/AOML dataset, both the PRR and PUV instruments collected profiles for certain wavebands (PAR and 380 nm). For stations where both instruments were deployed, data for these wavebands from the different instruments were considered replicates. As there were no instances of concurrent in situ data from any of the four data sources, no attempts were made to identify or reconcile any differences between instruments as they pertain to calibration or performance.

3.2 Satellite data collection

All MODIS/A Level-1A data from the Florida Keys region and within the years 2002–2012 (4566 files) were downloaded from the NASA Goddard Space Flight Center (GSFC) ocean color website http://oceancolor.gsfc.nasa.gov. Only MODIS/A data were used due to the stripping and scan mirror damage on MODIS/Terra, which limited its utility for ocean color research (Franz, Kwiatkowski, Meister, & McClain, 2008). Using default processing parameters and SeaDAS version 6.4, level-2 RSG at all visible bands (412, 443, 469, 488, 531, 547, 555, 645, 665, and 678 nm), as well as the level-2 processing flags, were created at 250 m resolution. For most MODIS bands, this spatial resolution was achieved by SeaDAS via interpolation from native 1 km or 500 m resolution. RSG data from each band were subsequently mapped to a cylindrical equidistant projection with bounds 24 to 26 N and 80 to 82 W, and stored in Hierarchical Data Format 4 (HDF4).

RSG data concurrent (i.e., same day and collocated) with in situ samples were extracted from these HDF4 files and stored in ASCII text.
files. MODIS data were removed from analysis if they were flagged by any of the standard level-2 processing flags (Patt et al., 2002). Also, any MODIS/A-derived spectrum with negative $R_{\text{bs}}$ at any wavelength was discarded to exclude any data with potential atmospheric correction failures. All image processing and data extraction were performed using IDL version 6.1 Interactive Data Language, Envisat Visual Information Solutions (IVIS). The concurrent satellite $R_{\text{bs}}$ and in situ measured water parameters that passed all quality control procedures are hereafter termed ‘matchups,’ while the matchup data from all parameters is the ‘training dataset.’ In total, concurrent MODIS/A $R_{\text{bs}}$ spectra were found for 74 of the 408 (18%) stations sampled, which represents the maximum possible number of matchups for any given parameter (number of matchups varies by parameter due to sampling differences between the two in situ data sources).

Once validated, the algorithm described below was applied to the entire time series of MODIS/A $R_{\text{bs}}$ in the Florida Keys region. Two locations, A (24.548°N, 81.397°W; Lower Keys) and B (24.651°N, 81.098°W; Middle Keys), were selected from within the FRT according to their repeated and long-term in situ sampling. Time series of derived water parameters were extracted for these two stations and binned by month. Image-wide monthly mean climatologies (2002–2012) of $K_{\alpha}(305)$ were also created for July and January to show representative summer and winter conditions, respectively. MODIS/A $R_{\text{bs}}$ from these two months were also processed to derive $K_{\alpha}(488)$ using the algorithm described by Barnes et al. (2013), from which monthly mean climatologies were calculated. Percent penetration of light to the benthos was calculated as:

$$P_{\text{penetration}}(z) = 10^{0.01\lambda z_{\text{bath}}},$$

where $z_{\text{bath}}$ is the bottom depth from a bathymetry database provided by the United States Geological Survey (USGS).

### 3.3 Algorithm development

Previously published variants of the EOF method often involved a cursory investigation of the shape of individual EOF modes to visually interpret how various water constituents might contribute to each mode (Craig et al., 2012; Fichot et al., 2008; Fischer et al., 1986; Toole & Siegel, 2001). Explaining the first two modes is typically straightforward, while subsequent modes require more conjecture. Despite the lack of apparent physical meaning, these subsequent modes may be most effective at representing the variance in the model (see von Storch & Zwiers, 1999). Measures of correlation to a concurrently measured water parameter have also been used to determine the contribution of water constituents to individual EOF modes (Fischer et al., 1986; Satyendranath et al., 1989, 1994; Toole & Siegel, 2001). When empirically modeling measured parameters, mode selection has previously included statistical justification using $R^2$ (Fichot et al., 2008); or confidence intervals of multiple regression coefficients (Craig et al., 2012; Mueller, 1976).

Mueller (1976) utilized different modes for estimation of different parameters. In contrast, while noting that certain EOF modes were negligibly contributing to the models for different parameters, Fichot et al. (2008) and Craig et al. (2012) used EOF modes 1–4 in the final models for all parameters to maintain consistency. In all of these works, only the first several (typically 4) modes were considered, owing to the high percentage of total variance (generally >90%) explained by these modes.

In this paper, we demonstrate the implementation of a stepwise, forward-addition procedure for selection of EOF modes to be retained for use in modeling water parameters. This approach reorders the guesswork and ambiguity from the EOF mode selection process. As such, statistically defensible mode selection is straightforward for model application to derive water parameters. Mueller (1976) and Craig et al. (2012) utilized multiple regression of EOF modes (aka principal components regression) to model water parameters. Our approach expands on this, while ensuring parsimony, through the forward addition of EOF modes (i.e., stepwise multiple regression).

As such, this process increases the statistical power of the multiple regression by including only independent variables that are significantly contributing to the explained variance of the dependent variable (Gauch, 1993). Inclusion of superfluous predictor variables will always increase the $R^2$ and Fisher’s test statistic (F) of a multiple regression (Cohen, Cohen, West, & Aiken, 2003). Although an EOF mode may explain a tiny portion of the total variance in $R_{\text{bs}}$, it may still be relevant in deriving water parameters (see von Storch & Zwiers, 1999).

Each water parameter was modeled independently using a modification of the EOF method. The term ‘parameter’ is used to describe $K_{\alpha}$, $a_{\alpha}$, or $a_{\beta}$ at a specific wavelength (for example, $K_{\alpha}(305)$ or $a_{\beta}(488)$), and there were 1939 parameters included in the training dataset. For each water parameter, only matchups with valid in situ data were included in the analyses. The number of matchups (N) varied by water parameter due to differences in sampling between the various projects from which data were collected and because of quality-control procedures. All water parameters were log-transformed to account for their approximtely log-normal distribution (Campbell, 1995). For simplicity, we will describe algorithm implementation for $K_{\alpha}(305)$, although all measured water parameters with matchup satellite $R_{\text{bs}}$ were analyzed in the same manner. All statistical analyses were performed using Matlab R2011a (Mathworks).

First, to focus on variability in spectral shape (as opposed to variability in amplitude), MODIS/A $R_{\text{bs}}$ spectra from $K_{\alpha}(305)$ matchups were normalized by:

$$R_{\text{bs}}(\lambda) = \frac{R_{\text{bs}}(\lambda)}{\int_{\alpha_{32}}^{\alpha_{34}} R_{\text{bs}}(\lambda) d\lambda},$$

where $R_{\text{bs}}(\lambda)$ is the normalized spectra (Craig et al., 2012). An EOF was then performed on the matchup MODIS/A $R_{\text{bs}}$, which partitioned the variance into the $K_{\alpha}(305)$ along 10 modes. Since the 10 visible MODIS bands were used in this analysis, these 10 modes explain 100% of the variance in the $R_{\text{bs}}$. The resulting scores for each of these EOF modes were used as the independent variables in a stepwise multiple regression (i.e., stepwise principal components regression), with the dependent variable being the matchup in situ $\log_{10}(K_{\alpha}(305))$. The significance of this global (i.e., all inclusive) model was tested using 1000 permutations. If the significance level of the global model was greater than alpha (0.05), no further analysis was performed to model or estimate this water parameter from MODIS/A data. However, if the global model was significant, stepwise multiple regression was further used to test the individual explanatory effect of each EOF mode on $\log_{10}(K_{\alpha}(305))$. A final model was constructed by sequentially adding the EOF modes to the model which resulted in the largest partial $F$. Addition of EOF modes to the model was stopped if addition of the next EOF mode raised either 1) the significance level over alpha or 2) the adjusted coefficient of multiple determination ($R^2_{\text{adj}}$) over that of the global model (see Blanchet, Legendre, & Borcard, 2008). This approach allows parsimonious determination of the EOF modes that are contributing to the variance in $K_{\alpha}(305)$. Coefficients of determination ($R^2$) in log-space are primarily used to describe the statistical relationships between these parsimoniously selected EOF modes and the matching in situ $\log_{10}(K_{\alpha}(305))$, hereafter termed ‘model’ results.

### 3.4 Predictive validation statistical methods

To test the ‘predictive’ ability of the approach, leave-one-out cross-validation was performed for each significant model result. To do so, multiple linear regression was performed, using only the significant EOF modes as independent variables and excluding data from one of the matchups. The EOF scores for the excluded matchup $R_{\text{bs}}$ were
then combined with the multiple linear regression coefficients to predict log$_{10}$(K$_d$(305)) for that matchup. This process was repeated N times, with each iteration excluding a different matchup. The predicted log$_{10}$ (K$_d$(305)) values were compared to the in situ measured log$_{10}$(K$_d$(305)) values using simple linear regression. Unbiased root mean squared percent error (URMS; Hooker, Ladin, Zibordi, & McLean, 2002) and bias of this predictive model were calculated on the non-transformed data as:

$$\text{bias} = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{\text{pred}_i - \text{meas}_i}{\text{meas}_i} \right)$$

and

$$\text{URMS} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{(\text{pred}_i - \text{meas}_i)^2}{\text{meas}_i^2} \right)}$$

where pred and meas represent predicted and measured values at i sample number. As a benchmark for URMS, the NASA mission goal for satellite-derived chlorophyll-a retrievals is 35% accuracy (Hooker, Esaias, Feldman, Gregg, & McClain, 1992). Gregg and Casey (2004) found Sea-viewing Wide Field-of-view Sensor (SeaWiFS) deSalt algorithms applied over global ocean waters show RMS greater than 0.2 for log transformed chlorophyll-a, which corresponds to relative RMS uncertainties over 58%.

4. Results

4.1. Model development and validation

A total of 1930 in situ parameters [e.g., K$_d$(305)] were tested using this approach, of which 1319 showed significant global models. In the following results and discussion, only results from K$_d$ and q$_d$ at 305 and 340 nm are described in detail. The rationale for the focus on these specific parameters is that they represent application of the approach in both the UVA (315–400 nm) and UVB (280–315 nm) wavelengths, which can lead to photoinduction and DNA damage, respectively (Lesser & Lewis, 1996; Zepp et al., 2000). While K$_d$ (and depth) determines the light exposure to the bacteria, q$_d$ is the dominant component of water absorption for blue and UV wavelengths in the FR region (Zepp et al., 2000). As an example, Fig. 3 shows the percentage contributions of particulate and dissolved matter absorption coefficients to the total non-water absorption coefficient at 440 nm. For most water samples, especially for those collected from the FRI, total non-water absorption is dominated by q$_d$ with minimal contributions from non-living detrital particles (a$_d$).

K$_d$ and q$_d$ at 305 and 340 nm all showed highly significant positive relationships between the in situ measurements and model results (Fig. 4). For K$_d$(305), 29 matchups were included in the training dataset with in situ values ranging from 0.28 to 3.27 m$^{-1}$. Regression of the model results and measured values (in log-space) showed an R$^2$ of 0.94, F of 438 and p-value < 0.01. K$_d$(304) showed very similar results across all statistical indices (N = 28; range = 0.17–2.23 m$^{-1}$; R$^2$ = 0.96; F = 527; p < 0.01). Strong positive relationships were also seen for q$_d$(305) (N = 65; range = 0.10–3.19 m$^{-1}$; R$^2$ = 0.87; F = 433; p < 0.01), and q$_d$(340) (N = 65; range = 0.02–1.50 m$^{-1}$; R$^2$ = 0.81; F = 271; p < 0.01), which had triple the number of matchups as K$_d$(UV), yet suffered little decrease in R$^2$.

The predictive ability of this approach, using leave-one-out cross-validation, showed slightly lower statistical performance than the model results (Fig. 5). Nevertheless, the regression of the prediction results with in situ values again showed strong positive relationships for K$_d$(305) (R$^2$ = 0.92; F = 314; p < 0.01; bias = −0.02 m$^{-1}$; URMS = 23%). K$_d$(340) (R$^2$ = 0.94; F = 386; p < 0.01; bias = −0.01 m$^{-1}$; URMS = 20%). Slightly lower R$^2$ and URMS were seen for q$_d$(305) (R$^2$ = 0.84; F = 320; p < 0.01; bias = −0.02 m$^{-1}$; URMS = 30%), and q$_d$(340) (R$^2$ = 0.74; F = 181; p < 0.01; bias = −0.01 m$^{-1}$; URMS = 46), yet the increased number of matchup data points greatly decreased the p-values for these parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model performance for selected parameters.</th>
</tr>
</thead>
<tbody>
<tr>
<td>K$_d$(305)</td>
<td>25</td>
</tr>
<tr>
<td>K$_d$(325)</td>
<td>25</td>
</tr>
<tr>
<td>K$_d$(340)</td>
<td>26</td>
</tr>
<tr>
<td>K$_d$(350)</td>
<td>54</td>
</tr>
<tr>
<td>K$_d$(410)</td>
<td>20</td>
</tr>
<tr>
<td>K$_d$(440)</td>
<td>22</td>
</tr>
<tr>
<td>K$_d$(490)</td>
<td>23</td>
</tr>
<tr>
<td>K$_d$(550)</td>
<td>23</td>
</tr>
<tr>
<td>K$_d$(670)</td>
<td>18</td>
</tr>
<tr>
<td>q$_d$(280)</td>
<td>40</td>
</tr>
<tr>
<td>q$_d$(305)</td>
<td>65</td>
</tr>
<tr>
<td>q$_d$(325)</td>
<td>65</td>
</tr>
<tr>
<td>q$_d$(340)</td>
<td>65</td>
</tr>
<tr>
<td>q$_d$(350)</td>
<td>63</td>
</tr>
<tr>
<td>q$_d$(410)</td>
<td>37</td>
</tr>
<tr>
<td>q$_d$(440)</td>
<td>40</td>
</tr>
<tr>
<td>q$_d$(490)</td>
<td>32</td>
</tr>
<tr>
<td>q$_d$(550)</td>
<td>35</td>
</tr>
<tr>
<td>q$_d$(670)</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 3
4.2. Application within the Florida Keys region

The application of any empirical algorithm should generally be restricted to the same spatiotemporal limits and range of environmental conditions as the training dataset. To accentuate this limitation, we have applied this approach to estimate $K_{u}(305)$ from satellite/in situ matchups (from the same data sources listed above) for waters adjacent to the FRT. Such retrievals yielded poor predictive relationships for both Straits of Florida (Fig. 6, open squares; $N = 9$; URMS = 126%) and Florida Bay (Fig. 6, open triangles; $N = 4$; URMS = 65%) waters. Incorporating the Straits of Florida matchups into the training dataset greatly improved the predictive performance of this approach (Fig. 6, closed squares; URMS = 70%). However, much less improvement was seen when Florida Bay waters were included in the training dataset (Fig. 6, closed triangles; URMS = 80%). The latter is likely due to the small number of matchups in this large and diverse region, but again highlights the need to limit application of this approach to the range of environmental conditions (e.g., water properties and bottom types) represented within the training dataset.

As such we have strived to incorporate in situ data spanning multiple years, with inclusion of data from all seasons and a variety of bottom types into our FRT training dataset. Further, the training dataset included a range of in situ values of at least one order of magnitude for most of the parameters being modeled and predicted. Nevertheless, the same logistical and financial limitations that plague established long-term monitoring programs hindered our ability to compile a training dataset that included all possible environments and water conditions (as well as combinations thereof) in the study area.

Such effect is also clearly seen when the developed model is applied to MODIS/A data to create a $K_{u}(305)$ map covering the entire Florida Keys region (Fig. 7, top panel). Even within the FRT, there appear to be locations for which $K_{u}(305)$ has not been properly derived. For example, in the shallow reefs (depths shallower than intertidal; Dustan & Halas, 1987) of the Upper Keys region, the spatial pattern in $K_{u}(305)$ appears to be associated with changes in depth. In the FRT, $K_{u}$ (on the scale of monthly climatologies) should instead decrease with distance to shore.

Fig. 3. Ternary plot showing percent contributions of water constituents CDOM, detritus, and phytoplankton pigments (i.e., non-water absorption coefficient at 440 nm for the FRT (red circles) and adjacent waters. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 4. Relationship between measured and modeled a) $K_{u}(305)$, b) $K_{u}(340)$, c) $a_{s}(305)$, d) $a_{s}(340)$. Solid line is 1:1 reference, while dotted lines show ±50% error.
and according to inundation from Florida Bay waters through channels between the islands (see Barnes et al., 2013). This effect of bottom contamination appears to be limited to waters shallower than 4.5 m. The training dataset used for this study includes locations just over 1 m deep, but such stations were primarily inshore as opposed to offshore, and the waters from these inshore stations were relatively turbid (i.e., less bottom contamination than for offshore clear water with the same water depth). This exclusion of extremely shallow, offshore, clear-water reef locations from the training dataset was primarily logistical (access by boat is limited due to the depth), but also due to quality control of the measured $K_d$ (reliable $K_d$ is difficult to measure in clear shallow waters due to the surface wave-focusing effect). Thus, we suggest limiting the application of the developed model to sites deeper than 4.5 m. This limit, however, does not represent a deficiency of the overall approach, and could be remedied with a more inclusive training dataset.

---

**Fig. 5.** Relationships between measured and predicted (via leave-one-out-cross-validation) a) $K_d$ (305), b) $K_d$ (340), c) $a_p$ (305), d) $a_p$ (340). Solid line is 1:1 reference, while dotted lines show ±50% error.

---

**Fig. 6.** Predictive performance of the SOR approach to derive $K_d$ (305) (m$^{-1}$) for waters in the Straits of Florida (squares) and Florida Bay (triangles). Open symbols show performance using only FRT data in the training dataset, while filled symbols represent retrievals when local samples are also included in the training dataset. Solid line is 1:1 reference, while dotted lines show ±50% error.
5. Discussion

5.1. Spatio-temporal variability of $K_d$ in the HRT

Within the HRT, excluding those noted regions where retrievals from the EOF model may be erroneous, the spatial changes in derived $K_d(305)$ appear to be reasonable. Specifically, a strong onshore-offshore gradient in $K_d(305)$ is apparent, which has also been described for $K_d(488)$ from MODIS/A data (Barnes et al., 2013), and is consistent with previous reports (Ayyub, 2009; Lapointe & Clark, 1992; Szmant & Forrester, 1996). $K_d(305)$ of the Upper, Middle, and Lower Keys regions also shows spatial patterns similar to the $K_d(488)$ patterns demonstrated by Barnes et al. (2013). However, there is a conspicuous difference in the seasonality of $K_d(305)$ and $K_d(488)$ (see below). Temporal patterns at individual locations have been validated by in situ measurements, suggesting the validity of the spatial $K_d(305)$ patterns and its temporal contrast with $K_d(488)$. For example, $K_d(305)$ time series at stations A and B derived for the entire span of MODIS/A measurements (Fig. 7, bottom graph) show $K_d(305)$ fluctuations that are verified by the occasional in situ data from these locations (note that these in situ data were not used in the training dataset due to lack of concurrent MODIS/A data). It is also worth noting that the largest peak in $K_d(305)$ for one of the time series (Middle Keys, Station B; Fig. 7) coincides with the January 2010 cold event in Florida (see Barnes & Hu, 2013; Barnes, Hu, & Muller-Karger, 2011; Liman et al., 2011), yea a similar peak was not seen in the Lower Keys time series (Station A). The $K_d(305)$ peak at Station B may be potentially attributed to cold event related die-offs of the Everglades fauna and subsequent CODM release.

Although the spatial patterns of $K_d(305)$ and $K_d(488)$ may be similar, their temporal changes can be drastically different. Fig. 8 shows monthly mean climatology (2002–2012) images of $K_d(305)$ and $K_d(488)$ for July and January to represent conditions for summer and winter, respectively. In these images, data from locations shallower than 4.5 m have been masked. If the shallow areas were completely surrounded by deeper water, $K_d$ data for the shallow areas were filled by interpolation from the adjacent deeper data. In the HRT, $K_d(488)$ is generally higher in the winter than in the summer (Fig. 8) via a regular seasonal cycle (Barnes et al., 2013). In contrast, $K_d(305)$ shows reversed temporal changes for much of the HRT, as seen in the July/January ratio images in Fig. 8. The higher $K_d(305)$ in July than in January is possibly driven by summer precipitation, which can lead to excessive CODM-rich terrestrial runoff. Increased CODM production from seagrass degradation is also expected in warmer waters (Stabinsen, Zepp, Bartsch, & Ziklo, 2004). Finally, even in dry summers, Everglades waters are occasionally released into Florida Bay to minimize adverse hypersalinity effects on seagrasses, providing another potential source of CODM in downstream HRT environments.

The contrast between the July/January ratios for $K_d(305)$ and $K_d(488)$ suggests that, unlike oligotrophic open-ocean waters where $K_d(305)$ is linearly proportional to $K_d(488)$ (Lee et al., 2013), the shallow Florida Keys waters are more optically complex and one cannot rely solely on $K_d$(VIS) to infer information on $K_d$(UV). This finding is not an artifact of differences between algorithms being used, as there was a great deal of scatter between concurrent $K_d$(VIS) and $K_d$(UV) retrievals when both were derived using the EOF approach.

Fig. 8 also highlights the much higher $K_d(305)$ than $K_d(488)$ throughout the HRT region. Consequently, the percent penetration of UV light to the benthos is much lower than that of blue light. In fact, the only locations with appreciable UV light reaching the benthos are the offshore shallow coral reef environments, especially in the Upper Keys region.

5.2. Potential use in coral reef assessment

In the context of coral reef research and monitoring, the potential uses of this long-term (2002–present), spatially synoptic dataset of UV
light penetration are numerous. Although the satellite measurement frequency is often semi-weekly due to cloud cover, the spatial and temporal coverage of this dataset is much higher than any in situ research and monitoring programs (e.g., 2 month repeat sampling for the NOAA AOML South Florida Program; see Kelble & Boyer, 2007). Thus, this new dataset could provide plentiful information with which to research the individual and combined effects of light and temperature on coral reefs in the FRT. In particular, a better understanding of the variation in UV light availability may help explain the distribution of corals away from tidal channels through the Keys (Ginsburg & Shinn, 1994, 1993), but seemingly contradictory success of nearshore reefs relative to offshore reefs (Lirman & Kong, 2007). Indeed, these offshore reefs are the only areas in the FRT for which appreciable levels of UV light reach the benthos. Thus, the offshore reefs may be more susceptible to the combined effects of UV and thermal oxidative stresses. However, there are complex interactions between water-column light absorption and temperature (e.g., radiative transfer) that confound a simple "either/or" explanation of UV and thermal stress on coral communities. Further, as reefs are often net exporters of CDOM (Boss & Zaneveld, 2003), these new products could be used to investigate the change in $K_d(UV)$ or $a_d(UV)$ for waters flowing over a reef, potentially providing insight into reef function. A thorough investigation of the direct and long-term impacts of satellite-derived SST and light availability on coral reef health in the Florida Keys is beyond the scope of this work.

The availability of long-term UV and visible light data in the Florida Keys allows for statistical assessment of the spatio-temporal patterns in light conditions within the FRT waters (see Section 5.1; Barnes et al., 2013). Such analyses can differentiate coral reef locations with distinct $K_d(UV)$ and $K_d(VIS)$ regimes, either according to mean condition or by annual or seasonal variability. The Florida Keys National Marine Sanctuary (FKNMS) is currently undergoing re-zonation of specific protection areas, in an effort to more effectively manage and protect the marine resources (NOAA, 2007, 2012). As with the $K_d(VIS)$ patterns, synoptic accounting of the UV light availability in the FRT and its effect on corals could be valuable in informing this rezoning process.

Beyond the FRT, the range of in situ values used in the training dataset and subsequently modeled using this approach are similar to other reported coral environments. Using $K_d(UV)$ as an example, our training fits within measurements reported by Dunn and Brown (1996), and Shick, Lesser, and Jokiel (1996), for a Maldives atoll lagoon ($K_d(UV) = 0.39 \text{ m}^{-1}$), Thailand coastal island ($K_d(UV) = 0.78 \text{ m}^{-1}$), Thailand inshore fringing reef ($K_d(UV) = 1.61 \text{ m}^{-1}$), Belize Barrier Reef ($K_d(UV) = 0.21 \text{ m}^{-1}$), Hawaii estuary ($K_d(UV) = 0.20 \text{ m}^{-1}$), and offshore Hawaii reef ($K_d(UV) = 0.20 \text{ m}^{-1}$). Also, the range of $K_d$ at 305, 320, 340, and 380 nm observed at coral reef locations surrounding Malaysia (Kwahara, Nakajima, Dhirman, Kohbari, & Toda, 2010) almost exactly matches the spread of the training dataset used in this FRT study. As such, beyond the general applicability of the approach to other environments, the particular parameterization of the models presented here may be directly applicable to coral reef environments worldwide.

5.3. Algorithm novelty — importance of stepwise model selection

While the use of EOF methods to derive water quality parameters such as $K_d$ is not new, the method presented here shows improvement over previously published EOF methods primarily through its implementation of the stepwise, forward addition procedure for selection of the EOF modes to be retained in the models. This approach allows for parsimonious and statistically defensible model selection for model application to the various measured parameters discussed in this paper as well as for application of this EOF method to any other region.

When applied to each of the in situ measured parameters, another important consequence of this new approach in implementing the EOF method is a ranking of the relative importance of the EOF modes.
in explaining variations in the parameter of interest. As seen in previous works (Craig et al., 2012; Fichot et al., 2009; Mueller, 1976), the mode selection varied not only by EOF or $K_d$ but also by wavelength within an EOF or $K_d$ (Fig. 9). In contrast to visual interpretation of the modes, this listing gives a more definitive indication of the meaning (in terms of effect on water parameter) of various portions of the eigenvectors (loadings by wavelength) for each mode (Fig. 10). For example, this analysis allows definitive assessment of mode 4 as representing changes in $R_{SP}$ according to $a_d$. Above approximately 550 nm, these changes are also concomitant with variability due to $a_d$. Further, low detrital contributions (Fig. 3) are confirmed by the modes most often selected for $a_d$ retrievals (4 and 9) which account for a total of 1.46% of the total variance in $R_{SP}$. Not surprisingly, $K_d$ retrievals do not generally include these modes, further highlighting the relatively small contributions of $a_d$ to total attenuation in the FIT.

It is important to note that most of the EOF modes discussed here are not ‘significant’ according to common selection rules (e.g., Rule N; Prekoodorfer, Zwers, & Barnett, 1982). Using the $K_3$305 matchups ($n = 29$) as an example, we performed 1000 EOF analyses on randomly generated noise (simulating 10 $R_{SP}$ bands for those 29 matchups). From these EOFs, we calculated the 95th percentile for the variance explained by each mode. As such, only mode 1 in our model explains more variance in $R_{SP}$ than would be predicted for random noise, and is thus ‘significant’ at $\alpha = 0.05$. However, this does not mean that subsequent modes are noise as predictors in the stepwise multiple regression. The forward selection process only includes independent variables that are significantly contributing to the variance in the dependent variable (in this case, log($K_3$305)), and the stopping procedures ensure parsimony. To demonstrate this, we have performed the stepwise multiple regression model for $K_2$305 data 1000 times, each with a different random (noise) predictor added to the 10 EOF modes. The noise variable was only selected in 53 cases (5.3%), very close to the acceptable significance level of the procedure.

In contrast, EOF mode 3 (a ‘non-significant’ mode that explains only 1.77% of the variance in $R_{SP}$) was selected in 99.3% of iterations.

5.4. Algorithm performance — resilience to instrument calibration uncertainties

As mentioned in the methods section, no attempts were made to quantify differences between performance of the various instruments used to collect the in situ data. The reason for this lack of intercalibration stems mostly from the fact that, due to the various data sources, instruments were not used concurrently. However, given the diversity of instrumentation used in the creation of the training dataset, the performance of the EOF model for predictions of many parameters indicates acceptable intercalibration errors between instruments. The EOF approach described here is also likely resilient to certain calibration errors or drift of the satellite instrument, mostly stemming from the stepwise procedure for model selection. EOF modes are included in the final model only if they parsimoniously explain a significant portion of the variance in the dependent variable. Although the few MODISA spectra with negative $R_{SP}$ (indicating failure of the atmospheric correction) were excluded from this analysis in an effort to have the most accurate possible training dataset, performance of the models did not generally suffer if such data were not excluded. As the normalization procedure (see Section 3.3; Craig et al., 2012) focuses on the spectral shape, negative $R_{SP}$ (which may have a physical meaning) may still carry some information useful in modeling water parameters.

More importantly, a slow drift of calibration errors in one or more of the satellite $R_{SP}$ bands could potentially be partitioned into one particular EOF mode. This is especially true if the matchups extend beyond the start of the instrument drift (i.e., some of the match $K_3$50 data are unaffected by the drift). Since the variation in the dependent variable is not likely to be explained by an EOF mode which has partitioned
the instrument drift, it is unlikely that the calibration error would be represented in the final model.

Actual conditions of the MODIS/A instrument blue bands (412 and 443 nm) allowed for testing of such resilience of this approach. Starting in early 2011, deterioration in these bands required a change in the radiometric calibration (Bryan Franz, NASA/GSFC, personal comm.). This change was implemented in SeaDAS version 6.4 but not in SeaDAS version 6.2. As such, by processing all MODIS/A data (especially from 2011 to 2012) with the outdated SeaDAS version 6.2, we were able to extract Rsun which included calibration drift in the 412 and 443 nm bands. These Rsun data were analyzed in the same manner as described above. Interestingly, most of the resulting EOF modes (and subsequent model performances) were quite similar to those from the SeaDAS version 6.4 processing (Fig. 10), with one exception being EOF mode 6, which explained 0.21% of the total variance in Rsun - Ks. This mode showed indications of seemingly random variance in all of the MODIS/A bands except those at 412 and 443 nm. For this mode, near-zero loadings in the blue bands could reflect stability relative to each other (i.e., improper calibration) independent of the variance in all other bands. Also, only 14 of the 1158 (1.23%) significant models (one mode for each parameter) included EOF mode 6 as parsimoniously explaining variance in that parameter. Given that EOF mode 6 showed a spectral shape that fits expectations for the instrument drift and generally does not explain in situ parameters, we conclude that EOF mode 6 likely partitioned the variance in Rsun associated with the instrument drift.

The resilience of the EOF model to instrument degradation or calibration uncertainties is particularly important to construct seamless environmental data records (EDRs) of Ks and aq using more than one satellite instrument. For example, at the time of this writing, MODIS/A exceeded its 5-year mission design by 6 years. In case of unexpected malfunction, the more recently launched Visible Infrared Imaging Radiometer Suite (VIIRS; 2011–present) and other future sensors (which may extend measurements to 340 or 350 nm; e.g., Fishman et al., 2012) may be used to continue the MODIS/A observations to form multi-decadal Ks and aq EDRs to address environmental problems associated with changing climate and increased anthropogenic activities.

6. Conclusions

The new approach in implementing the EOF method developed in this study improves over its predecessors in its requirements for parsimonious model selection. The method has been applied directly
to satellite-derived Rrs data, with validation procedures designed to estimate performance of its prediction capacity. The approach should be applicable to other regions, although performance is limited by the bounds of the training dataset. The success of the approach to derive Ks(UV) and a(UV) for a large dynamic range in the study region shows its applicability in optically shallow environments and outside the range of the measured Rrs. The contrasting seasonal changes in Ks(UV) and Ks(VIS) suggest that the former cannot be derived from the latter through spectral extrapolation or empirical regression, as they may be controlled by different forces. The contrast also highlights the need for more research and monitoring of the long-term and large-scale effects of UV light reaching the shallow-water benthos. The established MODIS-Aqua based long-term Ks(UV) EER makes such research possible, especially when combined with other environmental variables such as SST and surface radiation.

Acknowledgements

This work was funded by the U.S. NASA through its Gulf of Mexico program, Ocean Biology and Biogeochemistry program, Decision Support program, and Water and Energy Cycle program. The authors wish to thank NOAA National Geophysical Data Center (Wissel & Smith, 1996) for providing coastline shapefiles, Florida Fish and Wildlife Conservation Commission’s Fish and Wildlife Research Institute for providing benthic habitat maps, USGS for providing bathymetry data, and NASA/GSFC Ocean Biology Processing Group (OBPG) for providing MODIS data and SeaDAS software, as well as two anonymous reviewers whose comments helped to greatly enhance this manuscript. Collection of its data was funded, in part, by NOAA-NURC subcontract No. 2004-198 and the U.S. Environmental Protection Agency Gulf Ecology Division Grant No. X7-5964(G007-0). Several coworkers work for the U.S. Environmental Protection Agency, but the views expressed in this article do not necessarily represent the views or policies of EPA. Mention of trade names, products, or services does not convey, and should not be interpreted as conveying, official EPA approval, endorsement or recommendation. Support for N. Meto was provided by NOAA’s AOML.

References


APPENDIX E:

USE OF LANDSAT DATA TO TRACK HISTORICAL WATER QUALITY

CHANGES IN FLORIDA KEYS MARINE ENVIRONMENTS

Use of Landsat data to track historical water quality changes in Florida Keys marine environments

Brian B. Barnes a,⁎, Chuanmin Hu a, Kara L. Holekamp b,c, Slawomir Blonski b,d, Bruce A. Spiering e, David Palandro f, Brian Lapointe g

a College of Marine Science, University of South Florida, 1407 7th Ave. South, St. Petersburg, FL 33710, USA
b Science Systems & Applications, Inc., Stennis Space Center, MS, USA
c Innovative Imaging & Research, Stennis Space Center, MS, USA
d Earth System Science Interdisciplinary Center, University of Maryland, College Park, MD, USA
e NASA Applied Science & Technology Project Office, Stennis Space Center, MS, USA
f Rosenstiel School of Marine and Atmospheric Science, University of Miami, Miami, FL, USA
g Harbor Branch Oceanographic Institute, Florida Atlantic University, Fort Pierce, FL, USA

ARTICLE INFO

Article history:
Received 4 June 2013
Received in revised form 18 September 2013
Accepted 17 September 2013
Available online 20 September 2013

Keywords:
Water quality
Remote sensing
Atmospheric correction
SeaWiFS

ABSTRACT

Satellite remote sensing has shown the advantage of water quality assessment at a spatial scale in coastal regions, yet modern sensors such as SeaWIFS or MODIS did not start until the late 1990s. To overcome the drawbacks of observations, only the Landsat series have the potential to detect major water quality events since the 1970s. However, such ability is hindered by the unknown data quality or consistency through time. Here, using the Florida Keys as a case study, we demonstrate an approach to identify historical water quality events through improved atmospheric correction of Landsat data and cross-validation with concurrent MODIS data. After aggregation of the Landsat-5 Thematic Mapper (TM) 30-m pixels to 240-m pixels (to increase the signal-to-noise ratio), a MODIS-like atmospheric correction approach using the Landsat surface reflective bands was developed and applied to the entire Landsat-5 TM data set from 1985 and 1995. Remote sensing reflectance (Rrs) anomalies from Landsat (2 standard deviations from a pixel-specific monthly climatology) were found to detect MODIS Rrs anomalies with over 90% accuracy for all three bands for the same period of 2002–2010. Extending this analysis for the entire Landsat-5 time-series revealed Rrs anomalies in the 1980s and 1990s, some of which are corroborated by known ecosystem changes due to changes in local freshwater flow. Indeed, TM Rrs anomalies were shown to be useful in detecting shifts in seagrass density, turbidity increase, black water events, and phytoplankton blooms. These findings have large implications for ongoing and future water quality assessment in the Florida Keys as well as in many other coastal regions.

© 2013 Elsevier Inc. All rights reserved.

1. Introduction

One of the challenges in remote sensing is placing measurements in the context of events before and after the life of an instrument. Several studies have compared the data of multiple satellite instruments in efforts to extend the time series of remotely sensed data (e.g., Maritorena & Siegel, 2005), occasionally finding significant disagreement in both time and space (e.g., Franz, 2003; Kowalczuk, 2009). Even so, temporal gaps exist during which little or no satellite data are available. For ocean color remote sensing, which has been shown to be particularly useful in assessing optical water quality of coastal waters, such a data gap exists after the Coastal Zone Color Scanner (CZCS) stopped functioning in early 1986 and before the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) was launched in late 1997.

Throughout this gap, however, satellites dedicated to land study continued to collect multi-spectral radiance data over coastal waters. The Landsat program began in 1972 and, through eight satellites, has maintained a nearly continuous record of satellite data for land and adjacent coastal waters. Landsat-5 (1984–2011) housed a Thematic Mapper (TM) sensor, which measured radiance with 30 m spatial resolution for 6 bands (three visible, three infrared), and thermal infrared (TIR) radiation at 120 m resolution. Each Landsat satellite has a polar orbit, crossing the equator at approximately 10:00 am local time with 185 km Earth-viewing swath width. As a result, repeat sampling time for a particular location occurs at 16-day intervals. Although its primary purpose is for use over land, Landsat data collected over coastal and inland waters have been used with varying success to detect features including eddies (Ahnais, Rooyer, & George, 1987), phytoplankton blooms (Hesslein, 1992), freshwater discharges (Lajudie, Mazze, & Clark, 1993), shallow algae (Hu, 2005), cyanobacteria blooms (Vincent et al., 2004), water quality (Decker & Peters, 1993; Giardina, Pepe, Brivio, Cerezi, & Zilli, 2001; Olmanson, Brue, & Brennecilii, 2006;
Wang, Xia, Fu, & Sheng, 2004), sea surface temperatures (Thomas, Byrne, & Weatherly, 2003), and coral community changes (Paladino, Andreoletti, Muller-Karger, & Hanan, 2001; Paladino et al., 2008), among others.

Since 2000 and 2002, respectively, the Moderate Resolution Imaging Spectroradiometers (MODIS) aboard the U.S. National Aeronautics and Space Administration (NASA) polar orbiting satellites Terra and Aqua (MODIS-T and MODIS-A) have provided near-daily measurements of radiance over the world's oceans after the CZCS (1978–1986) and SeasWiFS (1997–2010) era. Most MODIS bands cover a spectral bandwidth of 10–20 nm with the spatial resolution of 250 m–1000 m. Aqua ascends across the equator at approximately 1:30 pm local time for daytime passes with a swath width of 2330 km, while Terra descends across the equator at 10:30 am local time with the same swath width. Despite significant differences in the spectral and spatial resolutions as well as in the signal-to-noise ratio (SNR) between MODIS and TM (Hu et al., 2012), similarities in their spectral band positions indicate the potential for filling the 1986–1997 historical data gap using Landsat TM. The satellites housing these instruments all orbit at an altitude of 705 km with nearly identical inclination (98.2° for Landsat 5, 98.14° for Aqua). The TM visible band centers (455, 560, and 660 nm for bands 1, 2, and 3) roughly correspond to those of MODIS bands 10, 4, and 13 (468, 555, and 667 nm; Fig. 1). For simplicity, these corresponding bands for both sensors are termed 'blue,' 'green,' and 'red,' respectively. Despite these similar band centers, there are large differences in spectral resolution between these bands (10–70 nm) and MODIS bands (10–20 nm). The narrower swaths width of the Landsat TM measurements (185 lm) every 16 days and the much wider swath of MODIS measurements (2330 km) every 1–2 days mean that nearly every Landsat image has a corresponding MODIS image on the same day. Although Terra coincides more closely with Landsat overpass times, significant residual errors due to striping and scan mirror damage limit MODIS data applicability for ocean color research (Franz, Kwiatkowska, Meister, & McClain, 2008). However, MODIS has provided quality data since 2002. It is therefore desirable to validate the quality and accuracy of Landsat TM data using concurrent MODIS data so that water quality data derived from MODIS-A can be extended to the 1980s.

Our approach to fill the 1986–1997 satellite ocean color gap through cross-validation of TM and MODIS data was motivated by several factors. First, MODIS ocean color bands were designed for research of water targets, while TM was intended for land assessment. As a result, achieving MODIS-quality data from TM imagery (rather than simply using TM data) is preferable for ocean color research. Second, cross-validation of TM with MODIS data will provide high-frequency (albeit low resolution) continuation and supplementation of the Landsat dataset. At the time of this research, Landsat 7 was in orbit, and Landsat 7 suffered a scan line corrector (SLC) failure. Although compromised Landsat 7 images can be used to measure water parameters (see D'Amore et al., 2008), the SLC failure effectively renders repeat sampling frequency. Landsat 8 includes an ocean color band in the blue, but it was only launched recently and its data were not available until 2013. MODIS data could serve as a bridge between these three sensors, and the regular overlap between MODIS and Landsat allows opportunities to assess instrument drift. This is in contrast to the cross-calibration between Landsat sensors, which is completed over a very short time window during which the instruments are placed in parallel orbits (see Tillet et al., 2001). Finally, the high repeat sampling frequency of MODIS sensors allows for creation of monthly or seasonal climatologies, which can be used to compare water quality events to the average condition over the last decade. Alone, the Landsat dataset lacks capacity to place elemental water quality features in the context of climatological norms due to the 16-day repeat sampling frequency. Proper cross-validation of these two sensors, however, would allow such assessment of TM detected events, which would significantly enhance our ability to study historical water quality events in coastal waters.

Extending MODIS observations in the 2000s to the 1980s and 1990s using Landsat TM, however, is technically challenging because of the sensor's differences in 1) band width and band positions; 2) radiometric calibration; 3) solar and viewing geometry; 4) SNR; and 5) overpass time. Although one may assume that the difference in their overpass time (2–3 h) may not result in significant changes in either the atmosphere or the water properties, and that the lower SNR in Landsat TM data may be increased by pixel binning, the first three issues must be adequately addressed. In order to use Landsat TM data in a similar fashion as with MODIS-A. Thus, in this study, an approach was developed to overcome the first three obstacles in order to make Landsat data comparable to MODIS and to subsequently assess historical water quality events. For demonstration of this application to use long-term Landsat TM data to study changes of the coastal ocean, we selected a delicate Florida Keys ecosystem that encompasses world renowned coral reefs, beaches, and seagrasses. Such analysis would provide information on the effects of Everglades water management and restoration practices on the water quality of downstream systems. Further, the ability to locate water quality events (in space and time) could provide a record of previous environmental stress and hint at resilience to future stresses for estuarine organisms. Specifically, the study had the following objectives:

1) To develop a practical method to construct long-term time series of atmospherically corrected Landsat TM data, validated for ocean color research.

2) To apply the dataset to identify historical water quality events in the Florida Keys ecosystem.

![Relative spectral response functions for Landsat TM bands (dashed) and MODIS-A bands (solid). Each color represents center wavelength for each band. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)](image-url)
2. Case study area – Florida Keys and surrounding waters

The Florida Keys is a 120 mile long archipelago of limestone islands located south of the Florida peninsula. Home to over 73,000 residents (US Census Bureau, 2011), these islands are a popular tourist destination with a population of approximately 2.5 million visitors annually generating nearly 1.2 billion dollars for the region (Casey, 2002). The waters surrounding the Florida Keys house a variety of shallow marine environments, including seagrass beds and coral reefs. Protection of these marine resources prompted the United States Congress in 1950 to create the Florida Keys National Marine Sanctuary (8ONMS), a 9000 km² marine protected area encompassing the Florida Keys.

Upstream of the Florida Keys marine ecosystems are the Florida Everglades, a subtropical wetland environment covering much of south Florida. Portions of the Everglades are also designated as protected areas, including the Big Cypress National Preserve and the Everglades National Park. The Shark and Caloosahatchee Rivers are major outflows of the Florida Everglades, leading into the Florida Keys region via Florida Bay and the Southwest Florida Bight (Fig. 2). Beginning in the early 1980s, due to concerns of hypersalinity affecting the marine ecosystems in Florida Bay and eutrophication of Lake Okeechobee, the Everglades Agricultural Area ceased pumping water runoff into Lake Okeechobee, instead diverting it to the riverine outflows. Although little data exist documenting the water quality of Florida Bay prior to the late 1980s, extremely clear water conditions were observed to be the norm (Fourqurean & Robbere, 1993; Stumpf, Prater, Durlak, & Brock, 1999). In the years since, the Florida Bay ecosystem has experienced large changes in water quality, concurrent with massive die-offs of seagrasses (Fourqurean & Robbere, 1993; Lapointe, Barile, & Matzie, 2004; Lapointe, Matzie, & Barile, 2002; Robbere et al., 1991; Stumpf, 1999). Much research suggests that increasing nutrient concentrations were responsible for seagrass decline in the Florida Keys region through eutrophication (Lapointe & Barile, 2004; Lapointe & Clark, 1993), competition with macroalgal species (Lapointe et al., 2002) or shading by phytoplankton blooms and increased turbidity (Lapointe & Clark, 1992; Lapointe et al., 2004; Phipps, 1C. L. & S. B., 1995). Although hypersalinity has also been proposed as a mechanism for seagrass decline (Robbere et al., 1991; Ziemann, Fourqurean, & Frankovich, 1999), the conclusion that hypersalinity caused the Florida Bay seagrass decline is questionable (National Research Council, 2002).

Smith and Pitts (2002) found net water flow from Florida Bay to the Atlantic Ocean side of the Florida Keys via tidal passes between the islands. As such, the water conditions in Florida Bay can impact the Florida Reef Tract (FRT), a string of bank reef environments south and east of the Florida Keys. Coral cover in the FRT has been in decline for several decades (Davies, 2000; Paladino et al., 2001, 2003; Porter et al., 2003) due in part to changes in water quality. Indeed, Lapointe et al. (2004) found anthropogenic enrichment of nitrogen is a key causal factor for the phytoplankton blooms on the FRT and subsequent declines in coral cover. Other factors which have been implicated in coral declines include overfishing (Ault, Rahbek, Smith, & Luo, 2005; Miller & Hay, 1998), phytoplankton blooms resulting from algal blooms (Leslie, Robertson, & Cobb, 1984), African dust (Garrison et al., 2003). Shinn et al., 2000), vessel groundings (Ebener, 2001), coral diseases (Porter et al., 2003), extreme temperature events (Jaap, 1985; Lirman et al., 2011; Warner, Fitt, & Schmidt, 1996), and water quality events (Hu, Muller-Karger, Vargo, Neely, & Johns, 2004; Hu et al., 2003; Zhao et al., 13).

For this study, four discrete locations were selected as representative examples of Florida Bay (A: 24.917°N, 81.08°W), Upper Keys (B: 24.97°N, 81.5°W) Middle Keys (C: 24.65°N, 81.14°W) and Lower Keys (D: 24.55°N, 81.56°W) waters (Fig. 2). Also, two transects were drawn

![Map showing the study region including bathymetry from National Geophysical Data Center coastal relief models. Seagrass environments (patchy and continuous, compiled using Florida Fish and Wildlife Research Institute data from 1987 to 2008) are shown in green, coral reefs (patchy and continuous) in red, land in black, and depth ranges in shades of blue. A, B, C, and D are locations used for time series analysis.](image-url)

Fig. 2. Map showing the study region including bathymetry from National Geophysical Data Center coastal relief models. Seagrass environments (patchy and continuous, compiled using Florida Fish and Wildlife Research Institute data from 1987 to 2008) are shown in green, coral reefs (patchy and continuous) in red, land in black, and depth ranges in shades of blue. A, B, C, and D are locations used for time series analysis.
to visualize spatiotemporal patterns. Within Florida Bay/SW Florida Bight, the transect was selected to maximize data coverage and span a variety of environments including seagrass and sponge beds. The second transect, south of the Florida Keys, captures patch and bank coral reef environments in addition to seagrass beds.

3. Methods — Data source and processing

Although CZCS provided satellite ocean color over the region between 1978 and 1986, it is unknown whether CZCS data could provide consistent data with modern sensors such as MODISA. In contrast, the long-term measurements of Landsat 5 TM (1984–2011) provide an opportunity to calibrate TM data using MODISA data, making it possible to extend recent observations to the 1980s and 1990s to form a continuous time series to the present. Towards this goal, Landsat 5 TM data were first processed using customized atmospheric correction to generate surface reflectance data (described below), which were then compared to concurrent MODISA reflectance data derived using a similar atmospheric correction approach. Confluent upon agreement between the sensors, MODISA data could be "back-casted" using historical TM data.

All Landsat 5 TM band 1–7 data from 1984 to 2010 for scenes (row–path) 015–043 and 016–043 (centering on the upper and lower Florida Keys, respectively) were obtained from the U.S. Geological Survey (USGS). Images with extensive cloud cover (approximately 75%) over the study area were excluded, leaving a total of 587 images with minimal cloud cover. The digital counts data were converted to top-of-the-atmosphere (TOA) radiance ($L_\lambda$, mW cm$^{-2}$ um$^{-1}$ sr$^{-1}$), then binned into groups of 64 ($\lambda$ = 0.4–0.8) in order to increase the SNR. The resulting data were thereby converted to 240 m resolution via neighborhood averaging. The maximum SNRs of these binned pixels are 8 times that of the original Landsat TM SNRs (72:1 in the blue to 29:1 in the red for typical radiances over the ocean; Hu et al., 2012), making them comparable to the SNRs of MODISA band bands. After atmospheric correction, the data were further binned to 1-km resolution, with a reduction in noise to further match the MODISA 1-km bands.

The atmospheric correction of MODISA is based on the principles and procedures detailed in Gordon and Wang (1994) and Gordon (1997), and then updated in Wang and Shi (2007). The sophisticated scheme derives the aerosol properties in the visible bands through extrapolation of the near-infrared (NIR) or shortwave-infrared (SWIR) measurements, and is embedded in the software package SeDAS (version 6.2 and higher). To assure consistency, a procedure similar to MODISA atmospheric correction has been implemented for Landsat. Although interested readers can refer to the published literature for the theoretical basis and detailed steps, for completeness of this paper the procedure is briefly described below.

For every image pixel, after correcting the gas absorption effects (in particular, ozone and water vapor) $L_\lambda$ is a result of the water-leaving radiation, $L_{\text{sw}}$, after propagating through the atmosphere and being superimposed on the atmospheric path radiance due to Rayleigh and aerosol scatterings ($L_{\text{a}}$ and $L_{\text{sw}}$):

$$L_{\lambda,\text{a}}(\theta) = L_{\lambda,\text{sw}}(\theta) + I_{\lambda,\text{a}}(\theta) + I_{\lambda,\text{sw}}(\theta),$$

(1)

where $\lambda$ is the wavelength, $\theta$ represents the solar-viewing geometry (solar zenith and sensor zenith angles and their relative azimuth), and $I_{\lambda,\text{a}}$ is the pixel-to-satellite diffuse transmittance at sensor zenith angle of $\theta$. Here, for simplicity, the contributions from whitecaps and sun glint are omitted. Once $L_{\lambda,\text{a}}$ is obtained from $L_{\lambda,\text{sw}}$, it is further converted to remote sensing reflectance ($R_{\lambda,\text{sw}}$, sr$^{-1}$) by:

$$R_{\lambda,\text{sw}} = L_{\lambda,\text{sw}}/f_{\lambda,\text{sw}} \cos(\theta_{\lambda}),$$

(2)

where $f_{\lambda,\text{sw}}$ is the diffuse transmittance from the sun to the pixel at the solar zenith angle of $\theta_{\lambda}$ and $f_{\lambda,\text{sw}}$ is the extraterrestrial solar irradiance adjusted for the sun-earth distance. $R_{\lambda,\text{sw}}$ is a fundamental parameter used for nearly all remote sensing inversion algorithms to estimate water quality parameters or benthic properties, and is the ultimate goal of atmospheric correction of satellite ocean color measurements.

For every image pixel, assuming negligible $L_{\text{sw}}$ or $L_{\text{a}}$ in the SWIR Landsat TM bands at 1.6 and 2.2 μm (SWIR1 and SWIR2, respectively), $L_{\lambda}$ in these bands is a result of atmospheric scattering and can be used to derive atmospheric path radiance and diffuse transmittance in other bands. In practice, the radiative transfer simulation software package MODTRAN4 (US Air Force Research Laboratory) was first used to determine Rayleigh scattering for each image-specific $\theta$, surface pressure, humidity, and ozone. Ancillary data from the National Centers for Environmental Prediction, Ozone Monitoring Instrument and Total Ozone Mapping Spectrometer were obtained to ascertain air pressure, relative humidity and ozone concentration for each individual scene.

MODTRAN was then used to estimate total and Rayleigh reflectance for two extreme aerosol types (maritime and tropospheric). Aerosol reflectance for these two aerosol types ($R_{\lambda,\text{sw}}^\text{Ray}$ and $R_{\lambda,\text{sw}}^\text{Mar}$, respectively) was estimated by subtracting Rayleigh from total reflectance. SWIR band ratios ($e$, $\delta$) were then calculated for all TM bands for both aerosol type conditions by:

$$\frac{\delta}{\delta_{\text{SWIR2}}} = \frac{R_{\lambda,\text{sw}}^\text{Mar}(\lambda, \text{SWIR2})}{R_{\lambda,\text{sw}}^\text{Trop}(\lambda, \text{SWIR2})}$$

(3)

and

$$\frac{\delta_{\text{SWIR1}}}{\delta_{\text{SWIR2}}} = \frac{R_{\lambda,\text{sw}}^\text{Mar}(\lambda, \text{SWIR1})}{R_{\lambda,\text{sw}}^\text{Trop}(\lambda, \text{SWIR1})}$$

(4)

The relationship between the SWIR1 band ratios from these extreme aerosol cases and that of the TM data ($e$) was calculated as:

$$e(\text{SWIR1}, \text{SWIR2}) = \frac{\delta_{\text{SWIR2}}}{\delta_{\text{SWIR1}}} = \frac{\delta_{\text{SWIR2}}}{\delta_{\text{SWIR1}}} \cdot \frac{\delta_{\text{SWIR1}}}{\delta_{\text{SWIR1}}},$$

(5)

This ratio was used to estimate aerosol $\varepsilon$ for the other TM bands as:

$$e(\lambda, \text{SWIR1}) = \left( \frac{\delta_{\lambda,\text{sw}}^\text{Trop}(\lambda, \text{SWIR1})}{\delta_{\lambda,\text{sw}}^\text{Trop}(\lambda, \text{SWIR2})} \cdot \frac{\delta_{\lambda,\text{sw}}^\text{Mar}(\lambda, \text{SWIR1})}{\delta_{\lambda,\text{sw}}^\text{Mar}(\lambda, \text{SWIR2})} \right) / e(\text{SWIR1}, \text{SWIR2})$$

(6)

Then, MODTRAN was used to estimate the atmospheric effects (path radiance and diffuse transmittance), finally resulting in $L_{\lambda}$ for each pixel. Note that although the concept of this atmospheric correction is identical to that used for MODISA ocean color measurements, there are two differences in their implementations. The first is that the spectral slope of aerosol scattering ($\varepsilon$) is defined here using multiple instead of single scattering. The second is that only two aerosol types are used to bracket the aerosol reflectance. This is analogous to the atmospheric correction of the 8-bit CZCS data (Gordon & Morel, 1983). Meanwhile the use of the SWIR bands of Landsat TM will minimize the potential contamination of the water signal to the total signal, making atmospheric correction easier for coastal waters.

The TM $L_{\lambda}$ data were then reprojected from their native Universal Transverse Mercator to a geographic latitude/longitude cylindrical projection where each pixel has 1 km resolution using bilinear interpolation. Although atmospheric correction was accomplished at 240 m resolution, 1 km resolution was used in order to reduce the image noise and to match the native resolution of the MODISA ocean color bands. Pixels with $L_{\lambda}$ above 0.05 sr$^{-1}$ in any wavelength were flagged as likely cloudy. To account for cloud shadow effects, an erosion operator was applied to these flagged TM pixels, meaning that the farthest extent of cloudy regions was widened by at least 1 km and subsequently removed from further analyses.
MODISA data from 2002 to 2010 and within the range 34° to 28° N, 89° to 69° W (a total of 2775 images) were downloaded from NASA Goddard Space Flight Center (GSFC). These data were processed using the standard atmospheric correction (SWIR and NIR combined; Wang & Shi, 2007) embedded in SeaDAS (version 6.2) to obtain \( R_{\text{TM}} \) for every MODISA band. Pixels determined to be cloudy by the CLDICE (cloud or ice-detected) algorithm (Duat et al., 2003) in level 2 processing flags (i.e., Rayleigh-corrected reflectance at 678 nm > 0.027) were removed from further analysis. The resulting \( R_{\text{TM}} \) data were also reprojected to the same geographic (latitude/longitude) cylindrical projection at 1 km resolution so data can be compared directly with Landsat \( R_{\text{LS}} \).

Land pixels (including a 1 km coastline) were excluded from all analyses, as were pixels outside the Florida Bay, Southwest Florida Bight and FLR regions. Image processing and analyses were performed using SeaDAS ENVI version 4.8 (Research Systems, Inc.) and IDL version 8.3 (ITT Visual Information Systems). Statistical metrics used in this analysis and TM atmospheric correction were performed using Matlab version R2011a (MathWorks).

4. Results and discussion

4.1. Cross-sensor agreement

Concurrent (within ~3 h) and collocated MODISA and TM \( R_{\text{LS}} \) measurements, hereby called ‘matchups’ (n), were extracted and compared by linear regression for all three bands. Positive linear trends described the relationships between the MODISA and TM data (Fig. 3a, green \( n = 201331, r^2 = 0.88 \); Fig. 3b, red \( n = 1106286, r^2 = 0.88 \); Fig. 3c) bands. The number of pixels differs for the three different bands due to negative \( R_{\text{LS}} \), especially in the red band.

Regardless of the high scattering, most of the data (>90% matchups) data density on the color legend) are centered around the 1:1 lines for all three bands, suggesting that the TM atmospheric correction and the potentials for using TM \( R_{\text{LS}} \) to extend MODISA \( R_{\text{LS}} \) to the 1980s and 1990s. Some of the large residuals, as well as discrepancies from the 1:1 line, likely resulted from the difference in spectral resolution (see Fig. 1). For example, the shortest wavelength with larger than 10% relative spectral response on the MODISA band 10 is 481 nm. In contrast, TM band 1 is largely unaffected by wavelengths less than 447 nm. Even though colored dissolved organic matter (CDOM) absorption affects \( R_{\text{LS}} \) for both of these wavebands, the effects of CDOM are larger in the shorter wavelengths. As the study region is typically CDOM rich, the linear regression slope of less than 1 between TM and MODISA \( R_{\text{LS}} \) matchups in the blue band is likely a result of the CDOM effect on the different bandwidths (Fig. 3a). Differences in the instrument radiometric calibrations, digitization bits (12 for MODIS, 8 for TM) and possibly SNRs, as well as insufficient cloud masking, may further explain some of the scatter in Fig. 3.

To visualize cross-sensor agreement over time, MODIS red, green, and blue \( R_{\text{LS}} \) data were averaged by month for several discrete locations (1 km pixels) throughout the study region. These data were plotted with Landsat TM \( R_{\text{LS}} \) from the same locations (Fig. 4). With the exception of some obvious outliers, there was generally strong agreement over time between the two sensors. True color TM imagery and MODISA imagery both show high turbidity events consistent with
most of the TM outliers, in these cases MODISA \( R_{\text{RS}} \) was also high, but not anomalous, nearby (in space and time) to the TM outliers, although this is obscured by monthly averaging in Fig. 4. Nevertheless, the relationship between TM and MODISA data appears to be consistent, with no apparent drift causing divergence of \( R_{\text{RS}} \) from the two sensors.

### Anomaly detection

MODISA data were used to create band-specific monthly \( R_{\text{RS}} \) climatologies for each calendar month using data from the years 2002–2010. The mean and standard deviation of all MODISA data at
each pixel were calculated. Normalized anomalies were subsequently created for all MODISA data by subtracting the image data from its pixel-specific monthly climatological mean, then dividing by the climatological standard deviation for that pixel. TM data were also rescaled to approximate MODISA values according to the band-specific linear regression equation (Fig. 5). As with the MODISA data, normalized anomalies (relative to the MODISA climatologies) were then created for the rescaled TM data.

These continuous normalized anomaly data were then classified categorically as either positive anomaly, negative anomaly, or no anomaly in order to highlight extreme anomaly events. For MODISA data, the threshold for this distinction was \( \pm 2.1 \) standard deviations (e.g., a pixel with normalized anomaly of \(-2.1\) was classified as negative anomaly). A stepwise (incrementally increasing by 0.1 standard deviations) approach was then taken to determine the positive and negative band-specific thresholds for categorial classification of TM anomalies based on the agreement with MODISA classifications. The final thresholds used in further analyses were the smallest (absolute) threshold with false positive rate (FPR) less than 0.05. This stepwise approach was necessary (as opposed to setting TM classification thresholds at \( \pm 2.1 \) standard deviations) in order to maximize the number of true positive detections while maintaining an acceptable false positive rate. F-measures (Witten & Frank, 2005) were calculated to assess the overall classification performance. F-measures are calculated from counts of true positives (TP), false positives (FP) and false negatives (FN) as \( \frac{2 \cdot TP}{TP + FP + FN} \). Note that since the goal is to measure the correct detection of anomalies, true negatives (TN) are not included in this metric.

The blue, green, and red band thresholds for positive TM Rg anomaly detection were 2.1, 1.8, and 2.3 standard deviations, while the thresholds for negative anomalies were –1.8, –1.5, and 1.5 standard deviations, respectively. F-measures for the positive anomalies were 1.08, 1.18, and 1.16, respectively, indicating strong performance of the TM positive anomaly detection. F-measures for the negative anomalies were lower (0.46, 0.21, and 0.12). The low F-measures for negative anomaly detection are due, in part, to fewer numbers of MODISA negative anomalies, which are by-products from the slowness of the MODISA data (see Fig. 3). Nevertheless, all anomaly classification methods showed greater than 90% accuracy. Tables 1, 2, and 3 show confusion matrices for TM positive and negative anomaly detections in the three bands. These thresholds were applied to all MODISA and TM data in order to create categorical anomaly data for the entire time series of both instruments. Fig. 5 shows an example of categorical anomalies detected by concurrent MODISA and TM on 1 February 2005. For every band, most spatial patterns of categorical anomalies agree between MODISA and TM, further suggesting cross-sensor consistency.

Given the acceptable performance of these anomaly detection methods, categorical anomaly data were extracted from all TM categorical anomaly images along the two transects in the study region (Fig. 6). For each 1 km pixel along these transects, the TM categorical anomaly data were extracted and dummy coded (−1 for negative anomaly, 0 for no anomaly, 1 for positive anomaly). Annual averages of the dummy coded data were subsequently plotted in time series (Fig. 6).

### Table 1

<table>
<thead>
<tr>
<th>MODISA condition (truth)</th>
<th>Positive anomaly</th>
<th>No positive anomaly</th>
<th>Negative anomaly</th>
<th>No negative anomaly</th>
</tr>
</thead>
<tbody>
<tr>
<td>TM positive anomaly</td>
<td>17016</td>
<td>18382</td>
<td>3369</td>
<td>9328</td>
</tr>
<tr>
<td>TM no positive anomaly</td>
<td>6557</td>
<td>162401</td>
<td>1926</td>
<td>179356</td>
</tr>
<tr>
<td>F-measure = 0.977</td>
<td>F-measure = 0.464</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>MODISA condition (truth)</th>
<th>Positive anomaly</th>
<th>No positive anomaly</th>
<th>Negative anomaly</th>
<th>No negative anomaly</th>
</tr>
</thead>
<tbody>
<tr>
<td>TM positive anomaly</td>
<td>18382</td>
<td>7977</td>
<td>1674</td>
<td>8864</td>
</tr>
<tr>
<td>TM no positive anomaly</td>
<td>5247</td>
<td>160849</td>
<td>1747</td>
<td>18446</td>
</tr>
<tr>
<td>F-measure = 1.175</td>
<td>F-measure = 0.211</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 3

<table>
<thead>
<tr>
<th>MODISA condition (truth)</th>
<th>Positive anomaly</th>
<th>No positive anomaly</th>
<th>Negative anomaly</th>
<th>No negative anomaly</th>
</tr>
</thead>
<tbody>
<tr>
<td>TM positive anomaly</td>
<td>14957</td>
<td>3900</td>
<td>362</td>
<td>4682</td>
</tr>
<tr>
<td>TM no positive anomaly</td>
<td>6524</td>
<td>84865</td>
<td>334</td>
<td>35586</td>
</tr>
<tr>
<td>F-measure = 1.362</td>
<td>F-measure = 0.123</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

As such, a pixel which showed negative anomaly for all images within a year (minimum 3 pixels required) would have a mean anomaly of \(-1\) (or \(100\%\)). As a result of the categorical classification and the 3 pixel per year minimum requirement, detected anomalies are only minimally affected by the sporadic outliers between MODIS and TM Rg (see Section 4.1). The first and most important conclusion to be drawn from Fig. 6 is that instrument drift is apparently not affecting the anomaly detections presented here. Even though the TM anomaly data are based on a MODISA climatology (2002–2010), there appear to be no regular trends in the derived anomalies. As a result, oscillations through time (as are expected in natural and impacted systems) are likely the result of changing environmental parameters. Specific anomalous reflectance events must be corroborated with historical events to infer their etiology.

4.3. Anomaly interpretation

Although there are some data gaps due to lack of sufficient data in the annual averages, the long-term space-time plots of TM-derived Rg anomalies between 1984 and 2010 show some coherent patterns in space and time (Fig. 6). For optically deep waters, the anomaly patterns in Rg can be attributed to changes in the concentrations of water constituents. Specifically, high suspended sediment loads would be represented by positive Rg anomalies in the red, green, and blue bands, while increased CDOM concentration would lower Rg in the blue band (Kirk, 1994). Phytoplankton blooms would similarly lower Rg in the blue band but increase Rg in the green band (Kirk, 1994).

In the Florida Keys region, however, the interpretation of anomalies is not as straightforward. Many of the waters in the region could switch from optically deep to optically shallow depending on the bottom depth, bottom type, and concentrations of the water constituents. Also, the bottom type is spatially and temporally variable, which can further complicate interpretation of the Rg anomalies. For instance, decreasing turbidity could cause Rg in the red band to decrease until the water becomes optically shallow. Then, further decreases in turbidity for optically shallow waters could result in an apparent increase in the red band Rg for a sandy (bright bottom) environment. Alternatively, a change in benthic albedo resulting from loss of seagrasses in an optically
shallow region could result in a similar (albeit likely more long term) \( R_g \) increase in both the green and red bands. As a result, a single large scale change in environmental parameters may be manifested in different (or even opposing) \( R_g \) signatures depending on the location or previous conditions.

Based on published literature describing the environmental changes in the study region (see Boyer & Jones, 2002; Durako, Hall, & Merello, 2002; Hall, Durako, Bourque, & Ziemann, 1999; Hu et al., 2003, 2004; Lapointe, Bedford, & Brumberger, 2007; Lapointe et al., 2004; Prager & Halley, 1999; Robbins et al., 1991; Stumpf et al., 1999;
Thayer, Murphey, & LaCroix, 1994) and on long-term river flow and wind speed data, below we attempt to interpret the RSG anomaly patterns created by landfast TM data in the three visible bands. Note that ideally, satellite-derived water quality parameters (water clarity or turbidity, chlorophyll-a concentration, COD absorption, etc.) would be used to determine the etiology of RSG anomalies. However, currently there is no reliable algorithm to convert TM RSG data to water quality parameters in such optically complex coastal environments. While future effort will be dedicated to such algorithm development, a qualitative interpretation of the RSG anomaly patterns is provided below for the two pre-selected transects. The agreement between TM-detected RSG anomalies and those predicted by known environmental changes serves as an indirect validation of the overall approach, and also sheds light on the larger spatiotemporal context of these environmental changes.

4.3.1. Florida Bay/Southwest Florida Bight

The most prominent features observed in the Florida Bay transect (Fig. 6) were anomalously high RSG events on the eastern end of the transect (east of 81.5 W). From the beginning of the time series to 1987, negative anomalies were seen in all three bands to the west of Florida Bay (approximate longitude 81.25 W, Fig. 6, circle 1). In 1988, these shifts to strongly positive anomalies which diminished in intensity around 1992 (Fig. 6, circle 2). Stumpf et al. (1999) found very similar trends in the red band reflectance at the same location using AVHRR data spanning the years 1985 to 1997. Specifically, Stumpf et al. (1999) showed “low reflectance in 1986–1987, high reflectance in 1988–1991, and low to moderate reflectance after that time” noting that the recovery of reflectance was “not quite to the reflectance range observed in 1986.” The change from low to high reflectance was attributed to seagrass die-offs beginning in 1987 (Robblee et al., 1991), while the subsequent return to previous RSG indicated “some increase in bottom cover” (Stumpf et al., 1999). Although in situ studies (Dutalco et al., 2002; Hall et al., 1999; Thayer et al., 1994) have not shown such increases of the dominant seagrass species (Thalassia testudinum) in this region, abundance of species adapted to lower light conditions (Halodule wrightii and Halodule englemanni) have increased in western Florida Bay (Dutalco et al., 2002).

Further, Stumpf et al. (1999) noted substantial increases in the red band reflectance within southwest Florida Bay (approximately 81 W, circle 3 in Fig. 6) starting in 1992 and continuing through the end of the study (1997). To our knowledge, the work by Stumpf et al. (1999) is the only long-term and spatially-synoptic investigation of water clarity and benthic cover in this region during the time gap without satellite ocean color coverage. The strong agreement between their results and the current study gives credence to the methodologies presented here, and justifies the wider (in space and time) interpretation of our findings. The current study expands on the results of Stumpf et al. (1999) by putting findings in a longer time context, while adding reflectance data for blue and green wavelengths.

Specifically, we find that the high reflectance in southwest Florida Bay (Fig. 6, circle 3) described as increased turbidity and/or loss of seagrasses by Stumpf et al. (1999) continued until at least 2001. After 2001, lack of TM data precluded continued assessment of this anomaly until 2005, at which point reflectance in northwest Florida Bay returned to previous (1984–1991) levels. Given the timing of these shifts compared to freshwater inputs to the region and the fact that these high anomalies were seen in all three TM bands, it is likely that turbidity is the main factor driving the high reflectance. Loss of seagrass cover may have exacerbated this turbidity by subjecting the benthos to greater wave energy (Prager & Halley, 1999), or may have contributed to the high RSG anomalies by exposing sandy benthos.

The South Florida Water Management District (SFWMMD) collects and maintains long-term datasets of daily flow rates for the Shark and Caloosahatchee Rivers (Fig. 7a). These data are continuous for both rivers from 1978 to present, and the average (1978–2010) annual combined river flow is 1.97 million acre-feet of water per year (afy). From 1984 to 1992, the mean was only 1.27 million afy. In contrast, the mean annual combined river flow from 1993–2005 was more than double (2.73 million afy) than that of the previous time span. Finally, the low flow condition was present again from 2006 to 2010, with the average annual combined river flow in this span at 1.27 million afy.

To illustrate the potential effects of these shifts in water flow regimes on the spatial extent of RSG changes in the region, mean anomaly images for each of these 3 time spans were created (Fig. 7b). These images highlight major changes in RSG, most notably in northwest Florida Bay (red arrows in Fig. 7b). In this region, low RSG anomalies in the low flow period are in stark contrast to widespread high anomalies in the wet period. As stated above, we find that changes in turbidity associated with these shifts in water flow regimes are likely the causative factor leading to the changes in red, green, and blue anomalies in the northwest Florida Bay.

In the western portion of the SW Florida Bight, a similar cycle of negative anomalies is seen (blue arrows in Fig. 7b), but only in the blue wavelengths. This region is relatively deep (20–30 m) and is not a seagrass habitat (see Fig. 2). The spectral composition of these anomalies is indicative of black water events which have been previously reported in the Florida Bight (Hu et al., 2003, 2004). Although the Florida Fish and Wildlife Conservation Commission regularly samples south Florida waters for the purposes of identifying and monitoring K. brevis (dinoflagellate red tide species) blooms, this region is surprisingly undersampled, and no such data were collected in this region of negative anomalies during the 1984–1992 time period. Unfortunately, in the absence of corroborating in situ data, we can only speculate on the etiology of this large region of negative anomalies during the 1984–1992 time period.

4.3.2. Florida Reef Tract

Compared to the Florida Bay transect, the RSG anomalies along the FRT transect are relatively minor and transient. Along the FRT transect, one notable feature is west of 82 W (Fig. 6, circle 4), where negative anomalies in the blue and green bands were common prior to 1992 (also seen in Fig. 7b, orange arrows). This region subsequently has seen regular blue-band anomalies, with green anomalies being more infrequent (Fig. 6). Despite abundant seagrasses, this area has been reported as having the highest chlorophyll concentration (Boyce & Jones, 2002) and diffuse attenuation coefficient (Barnes et al., 2013) in the FRT region owing to nutrient inputs from Florida Bay and the SW Florida Bight. Since these anomalies are based on the mean and standard deviation climatologies at each pixel, this feature does not describe spatial differences in RSG along the reef tract. Instead, this feature likely indicates a loss or thinning of seagrass coincident with the beginning of the 1992–2006 wet period. The elevated nutrient concentrations in waters advected from Florida Bay could cause eutrophication or shading by increases in phytoplankton blooms (Lepoint et al., 2004, 2007). Lack of data in the red band makes further interpretation difficult.

Positive anomalies were seen for all three TM bands along the FRT in 1998 (Fig. 6, circle 5). True color Landsat images show extreme turbidity events which covered the FRT in March, April and November 1998. SVMFMD data show that combined Caloosahatchee and Shark river discharge was high in 1998 (3.3 million afy), however such positive RSG anomalies and large scale extreme turbidity events were not seen in the FRT for other high flow years. Hourly wind data collected by the National Data Buoy Center (NDBC) stations in the region show above-average wind speed in the FRT preceding the turbidity events in March and April, but not in November. Nevertheless, these large scale turbidity events undoubtedly reduced the light available to benthic habitats. Such turbidity could have detrimentally impacted FRT coral environments via sedimentation (see Rogers, 1990). It is worth noting that due to extremely high temperatures resulting from El Niño conditions, mass bleaching of coral tissue was observed globally in summer 1998 (Hoegh-Guldberg, 1999). This mass bleaching did not contribute to the positive mean RSG anomalies along the FRT transect in 1998, as
the only summertime TM scene from 1996 did not show such positive anomalies.

Less intense, but similarly widespread R46 positive mean anomalies were seen along the FRT in 1985 and 1991 (Fig. 6, not circled). For both years, TM true color images show turbidity events in the first three months of the year. Unlike the turbidity events observed in 1996, however, the turbidity in 1985 and 1991 does not visually appear to be characteristic for wintertime images. Nevertheless, this analysis indicates that these events resulted in R46 anomalies, indicating severity of events which is not discernable from visual interpretation of the TM imagery. Very low combined Caloosahatchee and Shark river flow was observed in both 1985 and 1991. NDOR buoy wind data coverage is extremely limited during these years, but land-based stations in Key West, FL (Key West International Airport and Key West Naval Air Station, data collected from NOAA National Climatic Data Center), showed typical wind patterns (speed and direction) in the early months of both 1985 and 1991. As demonstrated for other R46 anomalies discerned from TM data in the region, such turbidity events can have detrimental effects on coral and seagrass environments (Green et al., 2004; Rogers, 1990).

Paladino et al. (2001, 2008) found changes in FRT coral cover using Landsat data, corroborated by field measurements. No such shifts are seen for the FRT in the current study for several reasons. First, the 1 km spatial resolution is too large to detect benthic albedo changes on the scale of coral cover loss in the FRT. Second, TM bands were analyzed individually as opposed to being used for benthic classification of pixels. As a result, subtle shifts in R46 spectra are not attributable to changes from coral to macroalgae-dominated environments.

4.4. General applications

Despite the preliminary success in establishing a MODISA-compatible Landsat TM time series for the study region, the use of Landsat data for interpretation of coastal waters and benthic environments in general requires caution. The low repeat sampling frequency can mean that large episodic events (e.g., hurricanes) may be underrepresented or missed completely. The paucity of TM data is exacerbated by clouds; the seasonality of which can result in a temporally biased dataset. For example, only two days in July 2002–2010 had both MODISA and Landsat 5 TM cloud-free data. This can have a potentially large effect on the validation of the anomaly detection methods. However, since the regression equations describing the relationship between MODISA/TM matchups did not vary greatly by month, we find application of the anomaly classification methods to be applicable to all months. Finally, the irregularity of cloud-free TM data can further affect the interpretation of the annual averages. At such, standardization of TM data to MODISA monthly reference climatologies was necessary to ameliorate this potentially confounding effect. Nevertheless, we have focused our interpretation of trends and events on anomalies that persist over many years or widespread scales, having been present in numerous satellite measurements. The resulting lack of temporal resolution for investigation of R46 anomalies is
offset by the increased confidence in the presence of noted events and trends.

Both MODISA and Landsat TM have global coverage. Thus, it is possible to extend the approach detailed here to other coastal regions in the world. This is because MODISA atmospherically corrected Rrs data are readily available from NASA, and with little effort the MODTRAN-based atmospheric correction can be applied to Landsat data from USGS. This may greatly facilitate studies to track water quality events in the 1980s and 1990s. In our study region, we found long term in situ datasets to be helpful in interpreting some of the observed Rrs anomalies, highlighting the importance of regular in situ environmental monitoring. However, such extraneous data are by no means required to conduct similar analyses of Rrs anomalies elsewhere. Indeed, the discoloration of TM Rrs anomalies with known water quality and benthic ecosystem changes was demonstrated here as an indirect validation of the methodology. We found that visual interpretation of the Landsat images, although useful in explaining observed Rrs anomalies, was not itself sufficient to detect certain events (e.g., seagrass density or composition changes), or to place events in the context of climatological norms (e.g., turbidity events). For example, in some cases, Rrs anomalies in the FRT were clearly attributable to turbidity events (i.e., visible in TM imagery). However, as similar turbidity events are also visible in TM imagery in years when no Rrs anomalies were detected, this approach allowed for the detection of the severity of such events, and thus their potential impact on the environment.

At the time of this writing, Landsat 5 has stopped functioning and Landsat 7 has missing data due to the SIC error. However, with an additional blue band, Landsat 8 began normal operations on 30 May 2013. The immediate next step is then to validate the consistency between Landsat 8 and MODISA during their overlapping period (i.e., after May 2013) so that Landsat 8 can provide continuous water quality observations in cases the already 12-year old MODISA failures.

5. Conclusions

The Landsat dataset presented here precedes the first reported major benthic environment shifts in the Florida Keys region, and provides a continuous 25 year record from which to analyze the spatial and temporal scales of these changes. In contrast to AVHRR data (see Stumpf et al., 1999), Landsat bands across the visible spectrum can be used to identify the specific etiology of Rrs anomaly events. As such, several large Rrs anomaly events, as measured by Landsat TM in the Florida Bay, have been identified and corroborated by previously documented events, including seagrass loss and turbidity increases. Many of the anomalies in Florida Bay Rrs coincide with periods of disparate water flow regimes from the Shark and Caloosahatchee Rivers.

This analysis indicates that large effects of freshwater flows in the Florida Bay are greatly muted in the FRT region. Although the linkage between Everglades discharge and nutrient enrichment of the FRT region has been established (Jayne et al., 2002, 2004, 2007), it is likely that the yearly averaging has obscured this connection. Indeed, primarily transient changes in yearly-averaged Rrs anomalies were noted south of the Florida Keys. However, previously unreported declines in seagrasses in the Marquesas Keys region appear to also coincide with the major increase in water flow to Florida Bay, and large turbidity events in 1998 appear to result primarily from high winds and riverine discharge.

Overall, this work highlights the need for wider spatial and temporal assessment of ecosystem changes, including water quality fluctuations as well as variations in coral health and seagrass density. Such changes in the environments of the Florida Keys appear to be significantly impacted by agriculture and management within the Everglades region. The impacts of proposed resource management actions must be better understood as they pertain to nutrient enrichment, hypersalinity, and the health of the downstream Florida Keys ecosystems. Likewise, the availability of global Landsat data, in combination with this newly proposed approach to assure multi-decadal data consistency, may greatly facilitate synoptic assessment of the coastal environments for much longer periods than enabled by modern satellite sensors starting from the late 1990s.

6. Acknowledgments

This work was supported by the U.S. National Aeronautics and Space Administration through its Decision Support program, Gulf of Mexico program, Ocean Biology and Biogeochemistry program, and Water and Energy Cycle program. Relative spectral response functions of Landsat TM and MODIS were provided by NASA. Shapefiles for seagrass and coral reef locations were provided by Florida Fish and Wildlife Research Institute. Landsat data and raster bathymetry were provided by the USGS. The authors wish to thank two anonymous reviewers whose critiques greatly improved this manuscript.

Reference


APPENDIX F:

AUTHOR CONTRIBUTIONS AND COPYRIGHT CLEARANCES

1. Author Contributions

Appendix A: An Improved High-Resolution SST Climatology to Assess Cold Water Events off Florida

B. B. Barnes developed approach, conducted analyses, and wrote manuscript

C. Hu and F. Muller-Karger developed approach and reviewed manuscript

Appendix B: A Hybrid Cloud Detection Algorithm to Improve MODIS Sea Surface Temperature Data Quality and Coverage Over the Eastern Gulf of Mexico

B. B. Barnes developed approach, conducted analyses, and wrote manuscript

C. Hu developed approach and reviewed manuscript

Appendix C: MODIS-derived spatiotemporal water clarity patterns in optically shallow Florida Keys waters: A New approach to remove bottom contamination

B. B. Barnes developed approach, collected data, processed data, conducted analyses, and wrote manuscript

C. Hu developed approach, acquired funding, and reviewed manuscript

B. A. Schaeffer and J. C. Lehrter acquired funding, collected data, processed data, and reviewed manuscript

Z. Lee developed approach and reviewed manuscript

D. A. Palandro acquired funding and reviewed manuscript

Appendix D: Estimation of diffuse attenuation of ultraviolet light in optically shallow Florida Keys waters from MODIS measurements

B. B. Barnes developed approach, collected data, processed data, conducted analyses, and wrote manuscript

C. Hu developed approach, acquired funding, and reviewed manuscript
J. P. Cannizzaro and R. Zepp collected data, processed data and reviewed manuscript

S. E. Craig and D. L. Jones developed approach and reviewed manuscript

P. Hallock and N. Melo collected data and reviewed manuscript

J. C. Lehrter and B. A. Schaeffer acquired funding, collected data, processed data, and reviewed manuscript

Appendix E: Use of Landsat data to track historical water quality changes in Florida Keys marine environments

B. B. Barnes developed approach, processed data, conducted analyses and wrote manuscript

C. Hu developed approach, acquired funding, and reviewed manuscript

K. L. Holekamp and S. Blonski processed data and reviewed manuscript

B. A. Spiering acquired funding, processed data and reviewed manuscript

D. A. Palandro acquired funding and reviewed manuscript

B. Lapointe reviewed manuscript
2. Copyright Clearances:

Appendices A and B:

Thesis / Dissertation Reuse

The IEEE does not require individuals working on a thesis to obtain a formal reuse license, however, you may print out this statement to be used as a permission grant:

Requirements to be followed when using any portion (e.g., figure, graph, table, or textual material) of an IEEE copyrighted paper in a thesis:

1) In the case of textual material (e.g., using short quotes or referring to the work within these papers) users must give full credit to the original source (author, paper, publication) followed by the IEEE copyright line © 2011 IEEE.
2) In the case of illustrations or tabular material, we require that the copyright line © [Year of original publication] IEEE appear prominently with each reprinted figure and/or table.
3) If a substantial portion of the original paper is to be used, and if you are not the senior author, also obtain the senior author’s approval.

Requirements to be followed when using an entire IEEE copyrighted paper in a thesis:

1) The following IEEE copyright/credit notice should be placed prominently in the references: © [year of original publication] IEEE. Reprinted, with permission, from [author names, paper title, IEEE publication title, and month/year of publication]
2) Only the accepted version of an IEEE copyrighted paper can be used when posting the paper or your thesis on-line.
3) In placing the thesis on the author's university website, please display the following message in a prominent place on the website: In reference to IEEE copyrighted material which is used with permission in this thesis, the IEEE does not endorse any of [university/educational entity's name goes here]'s products or services. Internal or personal use of this material is permitted. If interested in reprinting/republishing IEEE copyrighted material for advertising or promotional purposes or for creating new collective works for resale or redistribution, please go to http://www.ieee.org/publications_standards/publications/rights/rights_link.html to learn how to obtain a License from RightsLink.

If applicable, University Microfilms and/or ProQuest Library, or the Archives of Canada may supply single copies of the dissertation.
Appendices C, D, and E:

Dear Brian:

Permission [to include articles in dissertation] is in fact covered by the rights you retain as an Elsevier journal author as outlined at http://www.elsevier.com/journal-authors/author-rights-and-responsibilities, which include inclusion in a thesis or dissertation, provided that proper acknowledgement is given to the original sources of publication. Permission extends to online publication of your dissertation provided that the Elsevier journal articles are not available for download as standalone PDFs but only embedded within the dissertation itself; this would not be considered “systematic distribution.” Should you require any further clarification or assistance, please let me know. Best of luck with your dissertation.

Regards,
Hop

Hop Wechsler
Permissions Helpdesk Manager
Global Rights Department
Elsevier
1600 John F. Kennedy Boulevard
Suite 1800
Philadelphia, PA 19103-2899
Tel: +1-215-239-3520
Mobile: +1-215-900-5674
Fax: +1-215-239-3805
E-mail: h.wechsler@elsevier.com

Questions about obtaining permission: whom to contact? What rights to request?
When is permission required? Contact the Permissions Helpdesk at:
+1-800-523-4069 x 3808    permissionshelpdesk@elsevier.com